

Supporting Information

Hückel Theory and Optical Activity

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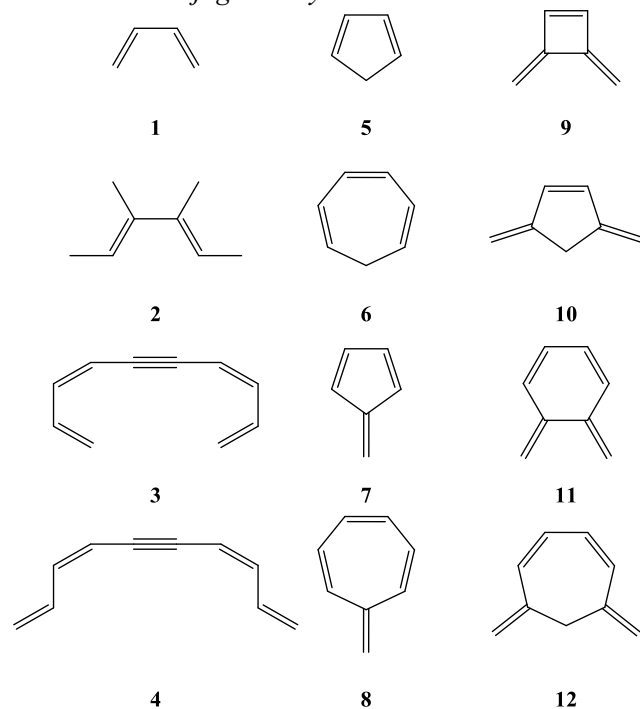
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S1. Full Gaussian Reference:

Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

S2. Planar Conjugated Hydrocarbon Structures:



S3. Number of Excited States Calculated

	6-311+G**	aug-cc-pVDZ
1	1635	1965
2	1767	2000
3	2000	2000
4	2000	2000
5	2000	2000
6	1107	1300
7	2000	2000
8	1372	1589
9	2000	2000
10	1107	1300
11	1372	1596
12	1808	2000

S4. Derivation of Equations:

Equation (7)

- Start with (1)

$$g_{\alpha\beta} = \frac{1}{4E} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} E (A_{\gamma\delta\beta} - A_{\delta\gamma\beta}) + \varepsilon_{\lambda\beta\gamma} G'_{\delta\lambda} - \varepsilon_{\lambda\beta\delta} G'_{\gamma\lambda} \right] \right\}$$

- Substitute (2) and (3)

$$g_{\alpha\beta} = \frac{1}{4E} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} E \left(2 \sum_{j \neq n} E_{jn} \operatorname{Re} \frac{\langle n | \mu_\gamma | j \rangle \langle j | \Theta_{\delta\beta} | n \rangle}{E_{jn}^2 - E^2} - 2 \sum_{j \neq n} E_{jn} \operatorname{Re} \frac{\langle n | \mu_\delta | j \rangle \langle j | \Theta_{\gamma\beta} | n \rangle}{E_{jn}^2 - E^2} \right) \right. \right. \\ \left. \left. - \varepsilon_{\lambda\beta\gamma} 2E \sum_{j \neq n} \operatorname{Im} \frac{\langle n | \mu_\delta | j \rangle \langle j | m_\lambda | n \rangle}{E_{jn}^2 - E^2} + \varepsilon_{\lambda\beta\delta} 2E \sum_{j \neq n} \operatorname{Im} \frac{\langle n | \mu_\gamma | j \rangle \langle j | m_\lambda | n \rangle}{E_{jn}^2 - E^2} \right] \right\}$$

- Factor out constants

$$g_{\alpha\beta} = \sum_{j \neq n} \frac{1}{2(E_{jn}^2 - E^2)} \left\{ \varepsilon_{\alpha\gamma\delta} E_{jn} \left[\frac{1}{3} (\operatorname{Re} \langle n | \mu_\gamma | j \rangle \langle j | \Theta_{\delta\beta} | n \rangle - \operatorname{Re} \langle n | \mu_\delta | j \rangle \langle j | \Theta_{\gamma\beta} | n \rangle) - \varepsilon_{\lambda\beta\gamma} \operatorname{Im} \langle n | \mu_\delta | j \rangle \langle j | m_\lambda | n \rangle \right. \right. \\ \left. \left. + \varepsilon_{\lambda\beta\delta} \operatorname{Im} \langle n | \mu_\gamma | j \rangle \langle j | m_\lambda | n \rangle \right] \right\}$$

- Substitute (5) and (6)

$$g_{\alpha\beta} = \sum_{j \neq n} \frac{1}{2(E_{jn}^2 - E^2)} \left\{ \varepsilon_{\alpha\gamma\delta} E_{jn} \left[\frac{1}{3} (V_{\gamma\delta\beta} - V_{\delta\gamma\beta}) - \varepsilon_{\lambda\beta\gamma} U_{\delta\lambda} + \varepsilon_{\lambda\beta\delta} U_{\gamma\lambda} \right] \right\}$$

- Substitute (4)

$$g_{\alpha\beta} = - \sum_{j \neq n} \frac{R_{\alpha\beta}^{jn}}{E_{jn}^2 - E^2}$$

Equation (8)

- Start with (1)

$$g_{\alpha\beta} = \frac{1}{4E} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} E (A_{\gamma\delta\beta} - A_{\delta\gamma\beta}) + \varepsilon_{\lambda\beta\gamma} G'_{\delta\lambda} - \varepsilon_{\lambda\beta\delta} G'_{\gamma\lambda} \right] \right\}$$

- Substitute (2) and (3) (simplify $\langle n | \mu_\alpha | j \rangle$ to μ_α , $\langle j | m_\alpha | n \rangle$ to m_α , and $\langle j | \Theta_{\alpha\beta} | n \rangle$ to $\Theta_{\alpha\beta}$)

$$g_{\alpha\beta} = \frac{1}{4E} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} E \left(2 \sum E_{n0} \frac{\mu_\gamma \Theta_{\delta\beta}}{E_{n0}^2 - E^2} \right) - 2 \sum E_{n0} \frac{\mu_\delta \Theta_{\gamma\beta}}{E_{n0}^2 - E^2} \right] - \varepsilon_{\lambda\beta\gamma} \left(2E \sum \frac{\mu_\delta m_\lambda}{E_{n0}^2 - E^2} \right) \right. \\ \left. + \varepsilon_{\lambda\beta\delta} \left(2E \sum \frac{\mu_\gamma m_\lambda}{E_{n0}^2 - E^2} \right) \right\}$$

- Factor out constants

$$g_{\alpha\beta} = \frac{1}{2} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} \left(\sum E_{n0} \frac{\mu_\gamma \Theta_{\delta\beta}}{E_{n0}^2 - E^2} \right) - \sum E_{n0} \frac{\mu_\delta \Theta_{\gamma\beta}}{E_{n0}^2 - E^2} \right] - \varepsilon_{\lambda\beta\gamma} \left(\sum \frac{\mu_\delta m_\lambda}{E_{n0}^2 - E^2} \right) + \varepsilon_{\lambda\beta\delta} \left(\sum \frac{\mu_\gamma m_\lambda}{E_{n0}^2 - E^2} \right) \right\}$$

- Simplify

$$g_{\alpha\beta} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{\alpha\gamma\delta} \left[\frac{1}{3} E_{n0} (\mu_\gamma \Theta_{\delta\beta} - \mu_\delta \Theta_{\gamma\beta}) - \varepsilon_{\lambda\beta\gamma} \mu_\delta m_\lambda + \varepsilon_{\lambda\beta\delta} \mu_\gamma m_\lambda \right] \right\}$$

Equation (12)

- For g_{zz} , substitute α subscripts with z and β subscripts with z

$$g_{zz} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{zy\delta} \left[\frac{1}{3} E_{n0} (\mu_\gamma \Theta_{\delta z} - \mu_\delta \Theta_{\gamma z}) - \varepsilon_{\lambda zy} \mu_\delta m_\lambda + \varepsilon_{\lambda z\delta} \mu_\gamma m_\lambda \right] \right\}$$

- Expand sum over all combinations of γ and cancel terms that become 0 because of repeating ε indicies.

$$g_{zz} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{zx\delta} \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{\delta z} - \mu_\delta \Theta_{xz}) - \varepsilon_{\lambda zx} \mu_\delta m_\lambda + \varepsilon_{\lambda z\delta} \mu_x m_\lambda \right] + \varepsilon_{zy\delta} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{\delta z} - \mu_\delta \Theta_{yz}) - \varepsilon_{\lambda zy} \mu_\delta m_\lambda + \varepsilon_{\lambda z\delta} \mu_y m_\lambda \right] + \cancel{\varepsilon_{zz\delta} [\dots]} \right\}$$

- Expand sum over all combinations of δ , cancel terms that become 0 because of repeating ε indicies, substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{zz} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \cancel{\varepsilon_{zxx} [\dots]} + \varepsilon_{zxy} \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{yz} - \mu_y \Theta_{xz}) - \varepsilon_{\lambda zx} \mu_y m_\lambda + \varepsilon_{\lambda zy} \mu_x m_\lambda \right] + \cancel{\varepsilon_{zxx} [\dots]} + \varepsilon_{zyx} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{xz} - \mu_x \Theta_{yz}) - \varepsilon_{\lambda zy} \mu_x m_\lambda + \varepsilon_{\lambda zx} \mu_y m_\lambda \right] + \cancel{\varepsilon_{zyy} [\dots]} + \cancel{\varepsilon_{zyz} [\dots]} \right\} g_{zz}$$

$$= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{yz} - \mu_y \Theta_{xz}) - \varepsilon_{yzx} \mu_y m_y + \varepsilon_{xzy} \mu_x m_x \right] - \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{xz} - \mu_x \Theta_{yz}) - \varepsilon_{xzy} \mu_x m_x + \varepsilon_{yzx} \mu_y m_y \right] \right\}$$

- Expand sum over all combinations of λ , cancel terms that will become 0 because of repeating ε indicies, substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{zz} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{yz} - \mu_y \Theta_{xz}) - \mu_y m_y - \mu_x m_x \right] - \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{xz} - \mu_x \Theta_{yz}) + \mu_x m_x + \mu_y m_y \right] \right\}$$

- Substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{zz} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ 2 \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{yz} - \mu_y \Theta_{xz}) - \mu_x m_x - \mu_y m_y \right] \right\}$$

- Simplify

$$g_{zz} = \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{yz} - \mu_y \Theta_{xz}) - \mu_x m_x - \mu_y m_y \right]$$

Equation (13)

- For g_{xy} , substitute α subscripts with x and β subscripts with y .

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{xy\delta} \left[\frac{1}{3} E_{n0} (\mu_\gamma \Theta_{\delta\gamma} - \mu_\delta \Theta_{\gamma\gamma}) - \varepsilon_{\lambda\gamma\gamma} \mu_\delta m_\lambda + \varepsilon_{\lambda y\delta} \mu_\gamma m_\lambda \right] \right\}$$

- Expand sum over all combinations of γ and cancel terms that become 0 because of repeating ε indicies.

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \cancel{\varepsilon_{xx\delta}} + \varepsilon_{xy\delta} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{\delta y} - \mu_\delta \Theta_{yy}) - \varepsilon_{\lambda yy} \mu_\delta m_\lambda + \varepsilon_{\lambda y\delta} \mu_y m_\lambda \right] \right. \\ \left. + \varepsilon_{xz\delta} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{\delta y} - \mu_\delta \Theta_{zy}) - \varepsilon_{\lambda yz} \mu_\delta m_\lambda + \varepsilon_{\lambda y\delta} \mu_z m_\lambda \right] \right\}$$

- Expand sum over all combinations of δ , cancel terms that become 0 because of repeating ε indicies, substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \cancel{\varepsilon_{xyx}} + \cancel{\varepsilon_{xyy}} + \varepsilon_{xyz} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \varepsilon_{\lambda yz} \mu_y m_\lambda \right] + \cancel{\varepsilon_{xzz}} \right. \\ \left. + \varepsilon_{xzy} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{yy} - \mu_y \Theta_{zy}) - \varepsilon_{\lambda yz} \mu_y m_\lambda + \varepsilon_{\lambda yy} \mu_z m_\lambda \right] + \cancel{\varepsilon_{xzz}} \right\}$$

- Expand sum over all combinations of λ , cancel terms that will become 0 because of repeating ε indicies, substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \varepsilon_{xyz} \mu_y m_x + \varepsilon_{yyz} \mu_y m_y + \varepsilon_{zyz} \mu_y m_z \right] \right. \\ \left. - \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{yy} - \mu_y \Theta_{zy}) - \varepsilon_{xyz} \mu_y m_x - \varepsilon_{yyz} \mu_y m_y - \varepsilon_{zyz} \mu_y m_z \right] \right\}$$

- Substitute 1 for ε_{xyz} , ε_{yzx} , and ε_{zxy} , and substitute -1 for ε_{xzy} , ε_{yxz} , and ε_{zyx} .

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \mu_y m_x \right] - \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{yy} - \mu_y \Theta_{zy}) - \mu_y m_x \right] \right\}$$

- Combine terms.

$$g_{xy} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ 2 \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \mu_y m_x \right] \right\}$$

- Simplify.

$$g_{xy} = \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \mu_y m_x \right]$$

- Repeat for g_{yx} .

$$\begin{aligned}
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{y\gamma\delta} \left[\frac{1}{3} E_{n0} (\mu_\gamma \Theta_{\delta x} - \mu_\delta \Theta_{\gamma x}) - \varepsilon_{\lambda x \gamma} \mu_\delta m_\lambda + \varepsilon_{\lambda x \delta} \mu_\gamma m_\lambda \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{yx\delta} \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{\delta x} - \mu_\delta \Theta_{xx}) - \varepsilon_{\lambda x x} \mu_\delta m_\lambda + \varepsilon_{\lambda x \delta} \mu_x m_\lambda \right] + \varepsilon_{yy\delta} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{\delta y} - \mu_\delta \Theta_{yy}) - \varepsilon_{\lambda y y} \mu_\delta m_\lambda + \varepsilon_{\lambda y \delta} \mu_y m_\lambda \right] \right. \\
&\quad \left. + \varepsilon_{yz\delta} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{\delta x} - \mu_\delta \Theta_{zx}) - \varepsilon_{\lambda x z} \mu_\delta m_\lambda + \varepsilon_{\lambda x \delta} \mu_z m_\lambda \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \varepsilon_{yxx} \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{zx} - \mu_z \Theta_{xx}) + \varepsilon_{\lambda x z} \mu_x m_\lambda \right] \right. \\
&\quad \left. + \varepsilon_{yzx} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) - \varepsilon_{\lambda x z} \mu_x m_\lambda + \varepsilon_{\lambda x x} \mu_z m_\lambda \right] + \varepsilon_{yyz} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zx} - \mu_z \Theta_{yy}) - \varepsilon_{\lambda y z} \mu_y m_\lambda + \varepsilon_{\lambda y x} \mu_z m_\lambda \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ - \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{zx} - \mu_z \Theta_{xx}) + \varepsilon_{\lambda x z} \mu_x m_\lambda + \varepsilon_{y x z} \mu_x m_y + \varepsilon_{z x z} \mu_x m_z \right] \right. \\
&\quad \left. + \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) - \varepsilon_{\lambda x z} \mu_x m_\lambda - \varepsilon_{y x z} \mu_x m_y - \varepsilon_{z x z} \mu_x m_z \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ - \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{zx} - \mu_z \Theta_{xx}) + \varepsilon_{y x z} \mu_x m_y \right] + \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) - \varepsilon_{y x z} \mu_x m_y \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ - \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{zx} - \mu_z \Theta_{xx}) + \varepsilon_{y x z} \mu_x m_y \right] + \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) - \varepsilon_{y x z} \mu_x m_y \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) + \mu_x m_y \right] - \left[\frac{1}{3} E_{n0} (\mu_x \Theta_{zx} - \mu_z \Theta_{xx}) - \mu_x m_y \right] \right\} \\
g_{yx} &= \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left\{ 2 \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) + \mu_x m_y \right] \right\} \\
g_{yx} &= \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) + \mu_x m_y \right]
\end{aligned}$$

- Take the average g_{xy} and g_{yx} .

$$g_{xy}^{symm} = \frac{1}{2} (g_{xy} + g_{yx})$$

- Substitute derived expressions of g_{xy} and g_{yx} .

$$g_{xy}^{symm} = \frac{1}{2} \left\{ \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} - \mu_z \Theta_{yy}) + \mu_y m_x \right] + \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_z \Theta_{xx} - \mu_x \Theta_{zx}) + \mu_x m_y \right] \right\}$$

- Simplify.

$$g_{xy}^{symm} = \frac{1}{2} \sum \frac{1}{E_{n0}^2 - E^2} \left[\frac{1}{3} E_{n0} (\mu_y \Theta_{zy} + \mu_z \Theta_{xx} - \mu_z \Theta_{yy} - \mu_x \Theta_{zx}) + \mu_x m_y + \mu_y m_x \right]$$

S5. Cartesian Coordinate System for 1:

Atom	x	y	z
C	0.00000	-1.54563	-0.50232
C	0.00000	-0.73516	0.56150
C	0.00000	0.73513	0.56149
C	0.00000	1.54563	-0.50232
H	0.00000	-2.62229	-0.38221
H	0.00000	-1.17184	-1.52076
H	0.00000	-1.19255	1.54790
H	0.00000	1.19260	1.54784
H	0.00000	1.17197	-1.52080
H	0.00000	2.62228	-0.38209

S6. Cartesian Coordinate System for 2:

Atom	x	y	z
C	-0.00002	0.75452	0.25054
C	-0.00001	-0.75452	0.25054
C	0.00000	1.46727	-0.89182
C	-0.00003	-1.46727	-0.89182
C	-0.00002	1.52283	1.56782
C	0.00003	-1.52283	1.56782
C	0.00003	2.98078	-1.03211
C	0.00001	-2.98078	-1.03211
H	0.00000	0.94473	-1.84293
H	-0.00006	-0.94473	-1.84293
H	-0.00022	0.88796	2.44804
H	-0.88005	2.16811	1.64477
H	0.88021	2.16782	1.64494
H	-0.00013	-0.88796	2.44804
H	0.88025	-2.16783	1.64491
H	-0.88000	-2.16811	1.64480
H	0.00014	3.50802	-0.07846
H	-0.87695	3.31661	-1.59947
H	0.87689	3.31658	-1.59966
H	0.00015	-3.50802	-0.07846
H	0.87686	-3.31657	-1.59968
H	-0.87698	-3.31662	-1.59945

S7. Cartesian Coordinate System for 3:

Atom	x	y	z
C	0.00000	-0.60957	1.17417
C	0.00000	0.60957	1.17417
C	0.00000	2.00020	1.39394
C	0.00000	-2.00020	1.39394
C	0.00000	3.03402	0.51334
C	0.00000	-3.03402	0.51334
C	0.00000	-3.04432	-0.94049
C	0.00000	3.04432	-0.94049
C	0.00000	1.99201	-1.77170
C	0.00000	-1.99201	-1.77170
H	0.00000	-4.03839	-1.38094
H	0.00000	-0.97621	-1.40494
H	0.00000	-2.13270	-2.84601
H	0.00000	-4.02028	0.96803
H	0.00000	-2.26970	2.44834
H	0.00000	2.26970	2.44834
H	0.00000	4.02028	0.96803
H	0.00000	4.03839	-1.38094
H	0.00000	0.97621	-1.40494
H	0.00000	2.13270	-2.84601

S8. Cartesian Coordinate System for 4:

Atom	x	y	z
C	0.00000	-0.60787	1.44408
C	0.00000	0.60787	1.44408
C	0.00000	2.01622	1.50411
C	0.00000	-2.01622	1.50411
C	0.00000	2.85982	0.44198
C	0.00000	-2.85982	0.44198
C	0.00000	-2.46331	-0.94894
C	0.00000	2.46331	-0.94894
C	0.00000	3.33041	-1.97246
C	0.00000	-3.33041	-1.97246
H	0.00000	2.44623	2.50226
H	0.00000	-2.44623	2.50226
H	0.00001	3.92692	0.64657
H	0.00001	-3.92692	0.64657
H	-0.00001	-1.39610	-1.15236
H	-0.00001	1.39610	-1.15236
H	0.00001	4.40334	-1.80722
H	0.00000	2.99314	-3.00187
H	0.00001	-4.40334	-1.80722
H	0.00000	-2.99314	-3.00187

S9. Cartesian Coordinate System for 5:

Atom	x	y	z
C	-0.00031	1.17934	-0.28177
C	0.00003	0.73422	0.99014
C	0.00020	-0.73404	0.99028
C	-0.00042	-1.17939	-0.28154
C	0.00034	-0.00012	-1.21600
H	-0.00046	2.21039	-0.60810
H	0.00016	1.34798	1.88192
H	0.00042	-1.34760	1.88219
H	-0.00064	-2.21050	-0.60769
H	-0.87638	-0.00016	-1.87796
H	0.87785	-0.00021	-1.87696

S10. Cartesian Coordinate System for 6:

Atom	x	y	z
C	0.00072	-1.28174	-0.97521
C	0.00044	-1.56515	0.34673
C	-0.00067	-0.67634	1.48896
C	-0.00058	0.67603	1.48913
C	0.00051	1.56505	0.34710
C	0.00066	1.28194	-0.97489
C	-0.00004	0.00019	-1.68498
H	0.00164	-2.14140	-1.64085
H	0.00110	-2.62177	0.59957
H	-0.00153	-1.16902	2.45670
H	-0.00134	1.16840	2.45699
H	0.00108	2.62159	0.60038
H	0.00136	2.14176	-1.64028
H	0.87298	0.00029	-2.30364
H	-0.96527	0.00023	-2.14674

S11. Cartesian Coordinate System for 7:

Atom	x	y	z
C	-0.00009	1.17833	0.12562
C	0.00006	0.73725	1.40378
C	0.00005	-0.73726	1.40377
C	-0.00008	-1.17833	0.12562
C	-0.00012	0.00000	-0.75994
C	0.00010	0.00000	-2.10193
H	-0.00018	2.20298	-0.21799
H	0.00019	1.35022	2.29522
H	0.00017	-1.35023	2.29521
H	-0.00016	-2.20297	-0.21803
H	0.00018	-0.92516	-2.66794
H	0.00018	0.92515	-2.66796

S12. Cartesian Coordinate System for 8:

Atom	x	y	z
C	0.00072	-1.28174	-0.57521
C	0.00044	-1.56515	0.74673
C	-0.00067	-0.67634	1.88896
C	-0.00058	0.67603	1.88913
C	0.00051	1.56505	0.74710
C	0.00066	1.28194	-0.57489
C	-0.00004	0.00019	-1.28498
C	-0.00097	0.00011	-2.64033
H	0.00164	-2.14140	-1.24085
H	0.00110	-2.62177	0.99957
H	-0.00153	-1.16902	2.85670
H	-0.00134	1.16840	2.85699
H	0.00108	2.62159	1.00038
H	0.00136	2.14176	-1.24028
H	-0.00143	0.92371	-3.20602
H	-0.00132	-0.92386	-3.20558

S13. Cartesian Coordinate System for 9:

Atom	x	y	z
C	-0.00001	-0.75684	-0.14023
C	0.00003	-0.67977	1.33890
C	-0.00003	0.67980	1.33889
C	0.00000	0.75685	-0.14023
C	0.00001	1.71329	-1.06583
C	-0.00001	-1.71332	-1.06579
H	0.00006	-1.42928	2.11916
H	-0.00004	1.42934	2.11913
H	0.00001	2.76268	-0.79393
H	0.00003	1.47203	-2.12241
H	0.00001	-2.76269	-0.79384
H	-0.00001	-1.47212	-2.12238

S14. Cartesian Coordinate System for 10:

Atom	x	y	z
C	0.00001	-1.20436	-0.11645
C	-0.00002	-0.67553	1.24400
C	-0.00001	0.67551	1.24402
C	0.00001	1.20437	-0.11639
C	-0.00003	0.00002	-1.05126
C	0.00004	-2.49710	-0.46810
C	0.00003	2.49710	-0.46810
H	-0.00003	-1.30664	2.12428
H	-0.00001	1.30655	2.12434
H	0.88075	0.00003	-1.69978
H	-0.88066	0.00004	-1.70000
H	-0.00001	-3.28255	0.27940
H	-0.00010	-2.80717	-1.50700
H	-0.00001	3.28259	0.27936
H	-0.00011	2.80710	-1.50702

S15. Cartesian Coordinate System for 11:

Atom	x	y	z
C	0.00002	0.74929	-0.62209
C	0.00003	-0.74929	-0.62212
C	0.00078	-1.41213	0.68084
C	0.00044	-0.72522	1.84115
C	-0.00055	0.72518	1.84116
C	-0.00072	1.41209	0.68088
C	0.00094	1.50330	-1.74281
C	-0.00096	-1.50323	-1.74287
H	0.00144	-2.49697	0.68376
H	0.00099	-1.25174	2.78898
H	-0.00092	1.25172	2.78898
H	-0.00112	2.49695	0.68384
H	0.00194	1.07992	-2.73877
H	0.00081	2.58481	-1.67631
H	-0.00214	-1.07984	-2.73884
H	-0.00086	-2.58474	-1.67640

S16. Cartesian Coordinate System for 12:

Atom	x	y	z
C	0.00315	-1.34913	-0.51710
C	0.00287	-1.63254	0.80484
C	0.00176	-0.74373	1.94707
C	0.00185	0.60864	1.94724
C	0.00294	1.49766	0.80521
C	0.00309	1.21455	-0.51678
C	0.00239	-0.06720	-1.22687
H	0.00078	-1.19710	2.87415
H	0.00105	1.06179	2.87442
H	0.00356	-2.63852	1.03512
C	0.04124	-2.37581	-1.38360
H	0.04258	-2.19390	-2.39944
H	0.06916	-3.34607	-1.03310
H	0.00373	2.50359	1.03570
H	-0.87189	-0.06715	-1.84374
H	0.96667	-0.06712	-1.69062
C	-0.02811	2.30542	-1.30123
H	-0.03090	2.20265	-2.32810
H	-0.04927	3.24582	-0.87671

*S17. Linear Response Gyration Tensor Output for 1 Using 6-311+G**:*

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-14.41	$\mathbf{G}'_{xy}/\omega$	50.51	$\frac{2}{3}\mathbf{A}_{xy}$	-27.37	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	12.76
$\mathbf{g}_{yx}$	-14.41	$\mathbf{G}'_{yx}/\omega$	0.09	$\frac{2}{3}\mathbf{A}_{yx}$	13.35	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-27.28
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	14.52
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	0.59
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-54.65
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zy}$	0.00

S18. Linear Response Gyration Tensor Output for 1 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-13.97	$\mathbf{G}'_{xy}/\omega$	45.81	$\frac{2}{3}\mathbf{A}_{xy}$	-30.30	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	10.17
$\mathbf{g}_{yx}$	-13.97	$\mathbf{G}'_{yx}/\omega$	1.28	$\frac{2}{3}\mathbf{A}_{yx}$	12.68	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-21.97
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	11.80
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-2.51
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-52.27

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
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S19. Linear Response Gyration Tensor Output for 2 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-17.44	$\mathbf{G}'_{xy}/\omega$	43.36	$\frac{2}{3}\mathbf{A}_{xy}$	-80.43	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	18.99
$\mathbf{g}_{yx}$	-17.44	$\mathbf{G}'_{yx}/\omega$	-0.98	$\frac{2}{3}\mathbf{A}_{yx}$	25.63	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-59.08
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	40.10
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-6.65
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-139.51
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00

S20. Linear Response Gyration Tensor Output for 2 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-16.35	$\mathbf{G}'_{xy}/\omega$	36.40	$\frac{2}{3}\mathbf{A}_{xy}$	-82.54	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	17.42
$\mathbf{g}_{yx}$	-16.35	$\mathbf{G}'_{yx}/\omega$	-0.40	$\frac{2}{3}\mathbf{A}_{yx}$	23.75	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-59.49
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	-0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	42.07
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-6.33
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-142.03

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00
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S21. Linear Response Gyration Tensor Output for 3 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.00	$\mathbf{G}'_{xx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$ 0.00
$\mathbf{g}_{xy}$ -135.06	$\mathbf{G}'_{xy}/\omega$ 503.63	$\frac{2}{3}\mathbf{A}_{xy}$ -102.10	$\frac{2}{3}\mathbf{A}_{y,xx}$ 0.00
$\mathbf{g}_{xz}$ 0.00	$\mathbf{G}'_{xz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$ 27.75
$\mathbf{g}_{yx}$ -135.06	$\mathbf{G}'_{yx}/\omega$ 8.27	$\frac{2}{3}\mathbf{A}_{yx}$ 45.43	$\frac{2}{3}\mathbf{A}_{x,yy}$ 0.00
$\mathbf{g}_{yy}$ 0.00	$\mathbf{G}'_{yy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$ 0.00
$\mathbf{g}_{yz}$ 0.00	$\mathbf{G}'_{yz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$ 34.77
$\mathbf{g}_{zx}$ 0.00	$\mathbf{G}'_{zx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$ 0.00
$\mathbf{g}_{zy}$ 0.00	$\mathbf{G}'_{zy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$ 0.00
$\mathbf{g}_{zz}$ 0.00	$\mathbf{G}'_{zz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$ -62.52
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -17.69
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$ -67.32
			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$ 0.00

S22. Linear Response Gyration Tensor Output for 3 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.00	$\mathbf{G}'_{xx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$ 0.00
$\mathbf{g}_{xy}$ -136.14	$\mathbf{G}'_{xy}/\omega$ 508.04	$\frac{2}{3}\mathbf{A}_{xy}$ -104.82	$\frac{2}{3}\mathbf{A}_{y,xx}$ 0.00
$\mathbf{g}_{xz}$ 0.00	$\mathbf{G}'_{xz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$ 30.06
$\mathbf{g}_{yx}$ -136.14	$\mathbf{G}'_{yx}/\omega$ 9.77	$\frac{2}{3}\mathbf{A}_{yx}$ 51.32	$\frac{2}{3}\mathbf{A}_{x,yy}$ 0.00
$\mathbf{g}_{yy}$ 0.00	$\mathbf{G}'_{yy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$ 0.00
$\mathbf{g}_{yz}$ 0.00	$\mathbf{G}'_{yz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$ 33.84
$\mathbf{g}_{zx}$ 0.00	$\mathbf{G}'_{zx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$ 0.00
$\mathbf{g}_{zy}$ 0.00	$\mathbf{G}'_{zy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$ 0.00
$\mathbf{g}_{zz}$ 0.00	$\mathbf{G}'_{zz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$ -63.90
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -21.26
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$ -70.98

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00
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S23. Linear Response Gyration Tensor Output for 4 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.00	$\mathbf{G}'_{xx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$ -0.00
$\mathbf{g}_{xy}$ -164.76	$\mathbf{G}'_{xy}/\omega$ 623.66	$\frac{2}{3}\mathbf{A}_{xy}$ -242.61	$\frac{2}{3}\mathbf{A}_{y,xx}$ 0.00
$\mathbf{g}_{xz}$ 0.00	$\mathbf{G}'_{xz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$ 171.94
$\mathbf{g}_{yx}$ -164.76	$\mathbf{G}'_{yx}/\omega$ 10.35	$\frac{2}{3}\mathbf{A}_{yx}$ 192.59	$\frac{2}{3}\mathbf{A}_{x,yy}$ 0.00
$\mathbf{g}_{yy}$ 0.00	$\mathbf{G}'_{yy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$ 0.00
$\mathbf{g}_{yz}$ 0.00	$\mathbf{G}'_{yz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$ -212.53
$\mathbf{g}_{zx}$ 0.00	$\mathbf{G}'_{zx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$ -0.00
$\mathbf{g}_{zy}$ 0.00	$\mathbf{G}'_{zy}/\omega$ -0.00	$\frac{2}{3}\mathbf{A}_{zy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$ 0.00
$\mathbf{g}_{zz}$ 0.00	$\mathbf{G}'_{zz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$ 40.59
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -20.65
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$ -455.14
			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$ 0.00

S24. Linear Response Gyration Tensor Output for 4 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.00	$\mathbf{G}'_{xx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$ 0.00
$\mathbf{g}_{xy}$ -166.40	$\mathbf{G}'_{xy}/\omega$ 621.87	$\frac{2}{3}\mathbf{A}_{xy}$ -253.63	$\frac{2}{3}\mathbf{A}_{y,xx}$ 0.00
$\mathbf{g}_{xz}$ 0.00	$\mathbf{G}'_{xz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{xz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$ 166.14
$\mathbf{g}_{yx}$ -166.40	$\mathbf{G}'_{yx}/\omega$ 12.67	$\frac{2}{3}\mathbf{A}_{yx}$ 191.54	$\frac{2}{3}\mathbf{A}_{x,yy}$ 0.00
$\mathbf{g}_{yy}$ 0.00	$\mathbf{G}'_{yy}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$ 0.00
$\mathbf{g}_{yz}$ 0.00	$\mathbf{G}'_{yz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{yz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$ -199.30
$\mathbf{g}_{zx}$ 0.00	$\mathbf{G}'_{zx}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zx}$ 0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$ -0.00
$\mathbf{g}_{zy}$ 0.00	$\mathbf{G}'_{zy}/\omega$ -0.00	$\frac{2}{3}\mathbf{A}_{zy}$ 0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$ 0.00
$\mathbf{g}_{zz}$ 0.00	$\mathbf{G}'_{zz}/\omega$ 0.00	$\frac{2}{3}\mathbf{A}_{zz}$ 0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$ 33.17
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -25.41
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.00
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 0.00
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$ -452.93

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
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S25. Linear Response Gyration Tensor Output for 5 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.01
$\mathbf{g}_{xy}$	-5.91	$\mathbf{G}'_{xy}/\omega$	22.78	$\frac{2}{3}\mathbf{A}_{xy}$	-1.43	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	-5.88
$\mathbf{g}_{yx}$	-5.91	$\mathbf{G}'_{yx}/\omega$	2.88	$\frac{2}{3}\mathbf{A}_{yx}$	5.47	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.02
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	-0.01	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-8.39
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.01
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	-0.02	$\frac{2}{3}\mathbf{A}_{zy}$	-0.01	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.01	$\frac{2}{3}\mathbf{A}_{z,zz}$	14.27
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-11.35
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.01
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-9.82
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00

S26. Linear Response Gyration Tensor Output for 5 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.01
$\mathbf{g}_{xy}$	-5.97	$\mathbf{G}'_{xy}/\omega$	21.03	$\frac{2}{3}\mathbf{A}_{xy}$	-4.53	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	-6.80
$\mathbf{g}_{yx}$	-5.97	$\mathbf{G}'_{yx}/\omega$	2.08	$\frac{2}{3}\mathbf{A}_{yx}$	2.96	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.01	$\mathbf{G}'_{yz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-5.58
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.01
$\mathbf{g}_{zy}$	0.01	$\mathbf{G}'_{zy}/\omega$	-0.02	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	12.38
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.02
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-9.76
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.01
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-10.11

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00
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S27. Linear Response Gyration Tensor Output for 6 Using 6-311+G:**

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	-0.00	$\mathbf{G}'_{xx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-1.27
$\mathbf{g}_{xy}$	-60.92	$\mathbf{G}'_{xy}/\omega$	243.6	$\frac{2}{3}\mathbf{A}_{xy}$	-3.78	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	-0.01	$\mathbf{G}'_{xz}/\omega$	0.03	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	-4.05
$\mathbf{g}_{yx}$	-60.92	$\mathbf{G}'_{yx}/\omega$	1.48	$\frac{2}{3}\mathbf{A}_{yx}$	6.68	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.44
$\mathbf{g}_{yy}$	-0.00	$\mathbf{G}'_{yy}/\omega$	-0.01	$\frac{2}{3}\mathbf{A}_{yy}$	-0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.21	$\mathbf{G}'_{yz}/\omega$	0.42	$\frac{2}{3}\mathbf{A}_{yz}$	-0.89	$\frac{2}{3}\mathbf{A}_{z,yy}$	11.41
$\mathbf{g}_{zx}$	-0.01	$\mathbf{G}'_{zx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.83
$\mathbf{g}_{zy}$	0.21	$\mathbf{G}'_{zy}/\omega$	-1.64	$\frac{2}{3}\mathbf{A}_{zy}$	0.14	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	-0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-7.36
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.30
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-10.73
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.06
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.01
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	7.63
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	-0.00

S28. Linear Response Gyration Tensor Output for 6 Using aug-cc-pVDZ:

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	-0.00	$\mathbf{G}'_{xx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-1.07
$\mathbf{g}_{xy}$	-60.87	$\mathbf{G}'_{xy}/\omega$	242.81	$\frac{2}{3}\mathbf{A}_{xy}$	-3.15	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	-0.01	$\mathbf{G}'_{xz}/\omega$	0.03	$\frac{2}{3}\mathbf{A}_{xz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	-5.45
$\mathbf{g}_{yx}$	-60.87	$\mathbf{G}'_{yx}/\omega$	0.29	$\frac{2}{3}\mathbf{A}_{yx}$	2.35	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.49
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	-0.01	$\frac{2}{3}\mathbf{A}_{yy}$	-0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.19	$\mathbf{G}'_{yz}/\omega$	0.49	$\frac{2}{3}\mathbf{A}_{yz}$	-0.90	$\frac{2}{3}\mathbf{A}_{z,yy}$	8.51
$\mathbf{g}_{zx}$	-0.01	$\mathbf{G}'_{zx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.59
$\mathbf{g}_{zy}$	0.19	$\mathbf{G}'_{zy}/\omega$	-1.56	$\frac{2}{3}\mathbf{A}_{zy}$	0.29	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	-0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-3.06
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.19
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.01
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-7.80
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.01
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.31
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.01
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$	5.36

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zy}$	-0.00
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S29. Linear Response Gyration Tensor Output for 7 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.01
$\mathbf{g}_{xy}$	-10.24	$\mathbf{G}'_{xy}/\omega$	36.90	$\frac{2}{3}\mathbf{A}_{xy}$	-30.29	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	22.49
$\mathbf{g}_{yx}$	-10.24	$\mathbf{G}'_{yx}/\omega$	-0.05	$\frac{2}{3}\mathbf{A}_{yx}$	22.09	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	27.60
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.01	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-50.08
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	0.39
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.02
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-2.70
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zy}$	0.00

S30. Linear Response Gyration Tensor Output for 7 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-10.12	$\mathbf{G}'_{xy}/\omega$	34.00	$\frac{2}{3}\mathbf{A}_{xy}$	-33.03	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	20.16
$\mathbf{g}_{yx}$	-10.12	$\mathbf{G}'_{yx}/\omega$	1.17	$\frac{2}{3}\mathbf{A}_{yx}$	22.44	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	30.19
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-50.35
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-2.28
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-2.83

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00
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S31. Linear Response Gyration Tensor Output for 8 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-0.03
$\mathbf{g}_{xy}$	-65.72	$\mathbf{G}'_{xy}/\omega$	240.74	$\frac{2}{3}\mathbf{A}_{xy}$	-81.45	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.01	$\mathbf{G}'_{xz}/\omega$	-0.03	$\frac{2}{3}\mathbf{A}_{xz}$	0.01	$\frac{2}{3}\mathbf{A}_{z,xx}$	37.84
$\mathbf{g}_{yx}$	-65.72	$\mathbf{G}'_{yx}/\omega$	5.41	$\frac{2}{3}\mathbf{A}_{yx}$	48.01	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.13
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.02
$\mathbf{g}_{yz}$	0.03	$\mathbf{G}'_{yz}/\omega$	-0.08	$\frac{2}{3}\mathbf{A}_{yz}$	0.01	$\frac{2}{3}\mathbf{A}_{z,yy}$	120.60
$\mathbf{g}_{zx}$	0.01	$\mathbf{G}'_{zx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.16
$\mathbf{g}_{zy}$	0.03	$\mathbf{G}'_{zy}/\omega$	-0.07	$\frac{2}{3}\mathbf{A}_{zy}$	-0.08	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.02
$\mathbf{g}_{zz}$	0.01	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-158.45
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.05
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-10.16
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.17
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.01
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	39.15
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.01

S32. Linear Response Gyration Tensor Output for 8 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-0.02
$\mathbf{g}_{xy}$	-65.35	$\mathbf{G}'_{xy}/\omega$	237.24	$\frac{2}{3}\mathbf{A}_{xy}$	-82.15	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.01	$\mathbf{G}'_{xz}/\omega$	-0.03	$\frac{2}{3}\mathbf{A}_{xz}$	0.01	$\frac{2}{3}\mathbf{A}_{z,xx}$	34.58
$\mathbf{g}_{yx}$	-65.35	$\mathbf{G}'_{yx}/\omega$	6.70	$\frac{2}{3}\mathbf{A}_{yx}$	47.22	$\frac{2}{3}\mathbf{A}_{x,yy}$	-0.12
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.02
$\mathbf{g}_{yz}$	0.03	$\mathbf{G}'_{yz}/\omega$	-0.07	$\frac{2}{3}\mathbf{A}_{yz}$	0.03	$\frac{2}{3}\mathbf{A}_{z,yy}$	118.76
$\mathbf{g}_{zx}$	0.01	$\mathbf{G}'_{zx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.14
$\mathbf{g}_{zy}$	0.03	$\mathbf{G}'_{zy}/\omega$	-0.07	$\frac{2}{3}\mathbf{A}_{zy}$	-0.06	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.02
$\mathbf{g}_{zz}$	0.01	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	-153.34
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	-0.06
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-12.64
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.18
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.01
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$	36.61

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.01
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S33. Linear Response Gyration Tensor Output for 9 Using 6-311+G:**

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-0.00
$\mathbf{g}_{xy}$	-9.69	$\mathbf{G}'_{xy}/\omega$	49.68	$\frac{2}{3}\mathbf{A}_{xy}$	-4.10	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	27.59
$\mathbf{g}_{yx}$	-9.69	$\mathbf{G}'_{yx}/\omega$	4.27	$\frac{2}{3}\mathbf{A}_{yx}$	34.50	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	-0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-57.72
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	30.14
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-6.92
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-61.83
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00

S34. Linear Response Gyration Tensor Output for 9 Using aug-cc-pVDZ:

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xx}$	-0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	-0.00
$\mathbf{g}_{xy}$	-9.62	$\mathbf{G}'_{xy}/\omega$	44.68	$\frac{2}{3}\mathbf{A}_{xy}$	-10.61	$\frac{2}{3}\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	24.32
$\mathbf{g}_{yx}$	-9.62	$\mathbf{G}'_{yx}/\omega$	6.01	$\frac{2}{3}\mathbf{A}_{yx}$	35.04	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	-0.00	$\mathbf{G}'_{yy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yy}$	-0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-51.76
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	27.44
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-10.72
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-62.36

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00
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S35. Linear Response Gyration Tensor Output for 10 Using 6-311+G:**

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-23.60	$\mathbf{G}'_{xy}/\omega$	98.07	$\frac{2}{3}\mathbf{A}_{xy}$	-11.56	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	13.90
$\mathbf{g}_{yx}$	-23.60	$\mathbf{G}'_{yx}/\omega$	3.91	$\frac{2}{3}\mathbf{A}_{yx}$	26.74	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yy}$	-0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.01	$\frac{2}{3}\mathbf{A}_{z,yy}$	-55.20
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{zy}$	-0.01	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.00
$\mathbf{g}_{zz}$	-0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	41.30
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-12.84
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-66.76
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	0.00

S36. Linear Response Gyration Tensor Output for 10 Using aug-cc-pVDZ:

$\mathbf{g}_{a\beta}$		$\mathbf{G}'_{a\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{a\beta}$		$\frac{2}{3}\mathbf{A}_{a,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{xx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-23.97	$\mathbf{G}'_{xy}/\omega$	96.02	$\frac{2}{3}\mathbf{A}_{xy}$	-17.25	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	12.47
$\mathbf{g}_{yx}$	-23.97	$\mathbf{G}'_{yx}/\omega$	3.95	$\frac{2}{3}\mathbf{A}_{yx}$	25.43	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}/\omega$	-0.00	$\frac{2}{3}\mathbf{A}_{yy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.01	$\frac{2}{3}\mathbf{A}_{z,yy}$	-51.14
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{zy}$	-0.01	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.00
$\mathbf{g}_{zz}$	-0.00	$\mathbf{G}'_{zz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,zz}$	38.67
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-12.96
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	0.00
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.00
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$	-68.40

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	-0.00
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S37. Linear Response Gyration Tensor Output for 11 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.03	$\mathbf{G}'_{xx}/\omega$	0.05	$\frac{2}{3}\mathbf{A}_{xx}$	-0.03	$\frac{2}{3}\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-80.21	$\mathbf{G}'_{xy}/\omega$	258.47	$\frac{2}{3}\mathbf{A}_{xy}$	-148.45	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	-0.00	$\mathbf{G}'_{xz}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	23.90
$\mathbf{g}_{yx}$	-80.21	$\mathbf{G}'_{yx}/\omega$	1.80	$\frac{2}{3}\mathbf{A}_{yx}$	27.31	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.03	$\mathbf{G}'_{yy}/\omega$	0.11	$\frac{2}{3}\mathbf{A}_{yy}$	0.09	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.01
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-52.28
$\mathbf{g}_{zx}$	-0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{zy}$	0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.01
$\mathbf{g}_{zz}$	0.07	$\mathbf{G}'_{zz}/\omega$	-0.03	$\frac{2}{3}\mathbf{A}_{zz}$	-0.06	$\frac{2}{3}\mathbf{A}_{z,zz}$	28.39
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.10
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-3.42
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.13
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.19
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$	-200.73
						$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	-0.00

S38. Linear Response Gyration Tensor Output for 11 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}/\omega$		$\frac{2}{3}\mathbf{A}_{\alpha\beta}$		$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.03	$\mathbf{G}'_{xx}/\omega$	0.06	$\frac{2}{3}\mathbf{A}_{xx}$	-0.04	$\frac{2}{3}\mathbf{A}_{x,xx}$	-0.00
$\mathbf{g}_{xy}$	-80.26	$\mathbf{G}'_{xy}/\omega$	254.88	$\frac{2}{3}\mathbf{A}_{xy}$	-152.19	$\frac{2}{3}\mathbf{A}_{y,xx}$	-0.00
$\mathbf{g}_{xz}$	-0.00	$\mathbf{G}'_{xz}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{xz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,xx}$	20.10
$\mathbf{g}_{yx}$	-80.26	$\mathbf{G}'_{yx}/\omega$	4.07	$\frac{2}{3}\mathbf{A}_{yx}$	28.01	$\frac{2}{3}\mathbf{A}_{x,yy}$	0.01
$\mathbf{g}_{yy}$	0.04	$\mathbf{G}'_{yy}/\omega$	0.10	$\frac{2}{3}\mathbf{A}_{yy}$	0.08	$\frac{2}{3}\mathbf{A}_{y,yy}$	0.01
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{yz}$	-0.00	$\frac{2}{3}\mathbf{A}_{z,yy}$	-46.16
$\mathbf{g}_{zx}$	-0.00	$\mathbf{G}'_{zx}/\omega$	0.00	$\frac{2}{3}\mathbf{A}_{zx}$	0.00	$\frac{2}{3}\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}/\omega$	0.01	$\frac{2}{3}\mathbf{A}_{zy}$	-0.00	$\frac{2}{3}\mathbf{A}_{y,zz}$	-0.01
$\mathbf{g}_{zz}$	0.07	$\mathbf{G}'_{zz}/\omega$	-0.03	$\frac{2}{3}\mathbf{A}_{zz}$	-0.04	$\frac{2}{3}\mathbf{A}_{z,zz}$	26.06
						$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$	0.00
						$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$	0.01
						$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$	-0.09
						$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$	-7.91
						$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$	-0.13
						$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$	-0.01
						$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$	-0.17
						$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$	-198.35

			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$	-0.00
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S39. Linear Response Gyration Tensor Output for 12 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.19	$\mathbf{G}'_{xx}/\omega$ -5.90	$\frac{2}{3}\mathbf{A}_{xx}$ 3.21	$\frac{2}{3}\mathbf{A}_{x,xx}$ 1.83
$\mathbf{g}_{xy}$ -189.72	$\mathbf{G}'_{xy}/\omega$ 669.49	$\frac{2}{3}\mathbf{A}_{xy}$ -223.43	$\frac{2}{3}\mathbf{A}_{y,xx}$ 20.76
$\mathbf{g}_{xz}$ -3.55	$\mathbf{G}'_{xz}/\omega$ 22.37	$\frac{2}{3}\mathbf{A}_{xz}$ 36.98	$\frac{2}{3}\mathbf{A}_{z,xx}$ 40.05
$\mathbf{g}_{yx}$ -189.73	$\mathbf{G}'_{yx}/\omega$ 1.95	$\frac{2}{3}\mathbf{A}_{yx}$ 48.47	$\frac{2}{3}\mathbf{A}_{x,yy}$ -0.39
$\mathbf{g}_{yy}$ -3.17	$\mathbf{G}'_{yy}/\omega$ -1.88	$\frac{2}{3}\mathbf{A}_{yy}$ -2.21	$\frac{2}{3}\mathbf{A}_{y,yy}$ -28.66
$\mathbf{g}_{yz}$ -0.52	$\mathbf{G}'_{yz}/\omega$ 0.01	$\frac{2}{3}\mathbf{A}_{yz}$ 1.86	$\frac{2}{3}\mathbf{A}_{z,yy}$ -170.60
$\mathbf{g}_{zx}$ -3.55	$\mathbf{G}'_{zx}/\omega$ -4.14	$\frac{2}{3}\mathbf{A}_{zx}$ -28.90	$\frac{2}{3}\mathbf{A}_{x,zz}$ -1.44
$\mathbf{g}_{zy}$ -0.52	$\mathbf{G}'_{zy}/\omega$ 1.14	$\frac{2}{3}\mathbf{A}_{zy}$ -3.68	$\frac{2}{3}\mathbf{A}_{y,zz}$ 7.90
$\mathbf{g}_{zz}$ -4.14	$\mathbf{G}'_{zz}/\omega$ 0.66	$\frac{2}{3}\mathbf{A}_{zz}$ -1.00	$\frac{2}{3}\mathbf{A}_{z,zz}$ 130.55
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ -8.13
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 3.29
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 3.80
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -8.42
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 7.00
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.42
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 6.01
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zy}$ -394.03
			$\frac{2}{3}\mathbf{A}_{z,yz}, \frac{2}{3}\mathbf{A}_{z,zv}$ -29.08

S40. Linear Response Gyration Tensor Output for 12 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$	$\mathbf{G}'_{\alpha\beta}/\omega$	$\frac{2}{3}\mathbf{A}_{\alpha\beta}$	$\frac{2}{3}\mathbf{A}_{\alpha,\beta\gamma}$
$\mathbf{g}_{xx}$ 0.33	$\mathbf{G}'_{xx}/\omega$ -6.08	$\frac{2}{3}\mathbf{A}_{xx}$ 3.40	$\frac{2}{3}\mathbf{A}_{x,xx}$ 1.77
$\mathbf{g}_{xy}$ -193.50	$\mathbf{G}'_{xy}/\omega$ 676.75	$\frac{2}{3}\mathbf{A}_{xy}$ -234.87	$\frac{2}{3}\mathbf{A}_{y,xx}$ 20.97
$\mathbf{g}_{xz}$ -3.64	$\mathbf{G}'_{xz}/\omega$ 22.95	$\frac{2}{3}\mathbf{A}_{xz}$ 37.66	$\frac{2}{3}\mathbf{A}_{z,xx}$ 34.91
$\mathbf{g}_{yx}$ -193.50	$\mathbf{G}'_{yx}/\omega$ 2.01	$\frac{2}{3}\mathbf{A}_{yx}$ 44.40	$\frac{2}{3}\mathbf{A}_{x,yy}$ -0.42
$\mathbf{g}_{yy}$ -3.31	$\mathbf{G}'_{yy}/\omega$ -1.61	$\frac{2}{3}\mathbf{A}_{yy}$ -2.24	$\frac{2}{3}\mathbf{A}_{y,yy}$ -29.12
$\mathbf{g}_{yz}$ -0.50	$\mathbf{G}'_{yz}/\omega$ -0.00	$\frac{2}{3}\mathbf{A}_{yz}$ 1.86	$\frac{2}{3}\mathbf{A}_{z,yy}$ -162.55
$\mathbf{g}_{zx}$ -3.64	$\mathbf{G}'_{zx}/\omega$ -4.34	$\frac{2}{3}\mathbf{A}_{zx}$ -29.54	$\frac{2}{3}\mathbf{A}_{x,zz}$ -1.35
$\mathbf{g}_{zy}$ -0.50	$\mathbf{G}'_{zy}/\omega$ 1.09	$\frac{2}{3}\mathbf{A}_{zy}$ -3.68	$\frac{2}{3}\mathbf{A}_{y,zz}$ 8.15
$\mathbf{g}_{zz}$ -4.14	$\mathbf{G}'_{zz}/\omega$ 0.58	$\frac{2}{3}\mathbf{A}_{zz}$ -1.16	$\frac{2}{3}\mathbf{A}_{z,zz}$ 127.64
			$\frac{2}{3}\mathbf{A}_{x,xy}, \frac{2}{3}\mathbf{A}_{x,yx}$ -8.57
			$\frac{2}{3}\mathbf{A}_{y,xy}, \frac{2}{3}\mathbf{A}_{y,yx}$ 3.27
			$\frac{2}{3}\mathbf{A}_{z,xy}, \frac{2}{3}\mathbf{A}_{z,yx}$ 3.53
			$\frac{2}{3}\mathbf{A}_{x,xz}, \frac{2}{3}\mathbf{A}_{x,zx}$ -9.49
			$\frac{2}{3}\mathbf{A}_{y,xz}, \frac{2}{3}\mathbf{A}_{y,zx}$ 6.92
			$\frac{2}{3}\mathbf{A}_{z,xz}, \frac{2}{3}\mathbf{A}_{z,zx}$ 0.50
			$\frac{2}{3}\mathbf{A}_{x,yz}, \frac{2}{3}\mathbf{A}_{x,zy}$ 5.76
			$\frac{2}{3}\mathbf{A}_{y,yz}, \frac{2}{3}\mathbf{A}_{y,zv}$ -397.42

			$\frac{2}{3}\mathbf{A}_{\text{L},\text{VZ}}, \frac{2}{3}\mathbf{A}_{\text{Z},\text{VZ}}$	-29.51
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S41. Sum-Over-All-State Gyration Tensors for 1 Using 6-311+G:**

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-14.59	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-23.69	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	-0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	-0.00	$\mathbf{A}_{z,xx}$	1.47
$\mathbf{g}_{yx}$	-14.59	$\mathbf{G}'_{yx}$	3.67	$\mathbf{A}_{yx}$	1.68	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	-60.68
$\mathbf{g}_{zx}$	-0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	-0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	-0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	5.61
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-0.21
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-84.37
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S42. Sum-Over-All-State Gyration Tensors for 1 Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-13.64	$\mathbf{G}'_{xy}$	0.09	$\mathbf{A}_{xy}$	-29.76	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	-0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.38
$\mathbf{g}_{yx}$	-13.64	$\mathbf{G}'_{yx}$	3.23	$\mathbf{A}_{yx}$	4.54	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	-0.00	$\mathbf{A}_{y,yy}$	-0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	-46.42
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	-0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	2.86
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	-0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	-0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-4.16
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-76.18

			$A_{z,yz}, A_{z,zy}$	-0.00
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S43. Sum-Over-All-State Gyration Tensors for 2 Using 6-311+G:**

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	0.02	$A_{x,xx}$	-0.00
g_{xy}	-17.50	G'_{xy}	-0.07	A_{xy}	-74.34	$A_{y,xx}$	0.00
g_{xz}	-0.00	G'_{xz}	-0.00	A_{xz}	0.00	$A_{z,xx}$	-12.54
g_{yx}	-17.50	G'_{yx}	3.28	A_{yx}	-1.60	$A_{x,yy}$	-0.01
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.01	$A_{y,yy}$	0.00
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	0.01	$A_{z,yy}$	-136.86
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	-0.01	$A_{x,zz}$	-0.00
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.01	$A_{y,zz}$	-0.00
g_{zz}	-0.00	G'_{zz}	-0.00	A_{zz}	-0.01	$A_{z,zz}$	14.26
						$A_{x,xy}, A_{x,yx}$	-0.01
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	-0.02
						$A_{x,xz}, A_{x,zx}$	-10.94
						$A_{y,xz}, A_{y,zx}$	0.00
						$A_{z,xz}, A_{z,zx}$	0.00
						$A_{x,yz}, A_{x,zy}$	-0.01
						$A_{y,yz}, A_{y,zy}$	-211.20
						$A_{z,yz}, A_{z,zy}$	-0.00

S44. Sum-Over-All-State Gyration Tensors for 2 Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	-0.00
g_{xy}	-15.73	G'_{xy}	0.00	A_{xy}	-81.80	$A_{y,xx}$	0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.01	$A_{z,xx}$	-9.09
g_{yx}	-15.73	G'_{yx}	2.63	A_{yx}	2.55	$A_{x,yy}$	0.01
g_{yy}	0.00	G'_{yy}	-0.00	A_{yy}	-0.00	$A_{y,yy}$	0.01
g_{yz}	0.01	G'_{yz}	-0.00	A_{yz}	0.00	$A_{z,yy}$	-130.51
g_{zx}	-0.00	G'_{zx}	-0.00	A_{zx}	-0.00	$A_{x,zz}$	0.00
g_{zy}	0.01	G'_{zy}	-0.00	A_{zy}	0.04	$A_{y,zz}$	-0.00
g_{zz}	-0.00	G'_{zz}	0.00	A_{zz}	0.00	$A_{z,zz}$	31.32
						$A_{x,xy}, A_{x,yx}$	-0.00
						$A_{y,xy}, A_{y,yx}$	-0.03
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-11.64
						$A_{y,xz}, A_{y,zx}$	0.00
						$A_{z,xz}, A_{z,zx}$	0.01
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	-212.30

			$A_{z,vz}, A_{z,vz}$	0.00
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*S45. Sum-Over-All-State Gyration Tensors for 3 Using 6-311+G**:*

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -132.51	G'_{xy} 0.46	A_{xy} -96.41	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} -0.00	$A_{z,xx}$ -10.92
g_{yx} -132.51	G'_{yx} 35.64	A_{yx} 11.13	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ 2.04
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -151.35
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -22.05
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -94.38
			$A_{z,yz}, A_{z,zy}$ 0.00

S46. Sum-Over-All-State Gyration Tensors for 3 Using aug-cc-pVDZ:

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -132.96	G'_{xy} 0.71	A_{xy} -97.93	$A_{y,xx}$ -0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} -0.00	$A_{z,xx}$ -9.76
g_{yx} -132.96	G'_{yx} 35.77	A_{yx} 22.61	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ -0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -6.61
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ -0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -150.87
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -32.36
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -104.54
			$A_{z,yz}, A_{z,zy}$ 0.00

			$A_{z,vz}, A_{z,zv}$	-0.00
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*S47. Sum-Over-All-State Gyration Tensors for 4 Using 6-311+G**:*

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ -0.00
g_{xy} -159.84	G'_{xy} 0.60	A_{xy} -72.74	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -4.09
g_{yx} -159.84	G'_{yx} 44.19	A_{yx} 21.17	$A_{x,yy}$ -0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ -0.00
g_{yz} -0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -592.62
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ -0.00
g_{zy} -0.00	G'_{zy} 0.00	A_{zy} -0.01	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -202.46
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -25.26
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -665.35
			$A_{z,yz}, A_{z,zy}$ 0.00

S48. Sum-Over-All-State Gyration Tensors for 4 Using aug-cc-pVDZ:

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ -0.00
g_{xy} -161.94	G'_{xy} 0.90	A_{xy} -109.15	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -5.55
g_{yx} -161.94	G'_{yx} 43.88	A_{yx} 32.18	$A_{x,yy}$ -0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} -0.00	A_{yz} -0.00	$A_{z,yy}$ -552.66
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} -0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -201.74
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -37.74
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ -0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -661.81
			$A_{z,yz}, A_{z,zy}$ 0.00

			$A_{z,yz}, A_{z,zy}$	0.00
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S49. Sum-Over-All-State Gyration Tensors for **5** Using 6-311+G**:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	-0.00	$A_{x,xx}$	0.01
g_{xy}	-6.02	G'_{xy}	0.21	A_{xy}	1.85	$A_{y,xx}$	-0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.01	$A_{z,xx}$	-10.63
g_{yx}	-6.02	G'_{yx}	1.74	A_{yx}	7.22	$A_{x,yy}$	-0.03
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	0.00	$A_{y,yy}$	-0.00
g_{yz}	0.01	G'_{yz}	-0.00	A_{yz}	-0.01	$A_{z,yy}$	-17.26
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	-0.00	$A_{x,zz}$	0.02
g_{zy}	0.01	G'_{zy}	-0.00	A_{zy}	-0.00	$A_{y,zz}$	0.01
g_{zz}	-0.00	G'_{zz}	-0.00	A_{zz}	-0.00	$A_{z,zz}$	22.51
						$A_{x,xy}, A_{x,yx}$	-0.00
						$A_{y,xy}, A_{y,yx}$	-0.03
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-17.85
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	0.00
						$A_{x,yz}, A_{x,zy}$	-0.00
						$A_{y,yz}, A_{y,zy}$	-15.41
						$A_{z,yz}, A_{z,zy}$	0.01

S50. Sum-Over-All-State Gyration Tensors for **5** Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	0.01	$A_{x,xx}$	0.02
g_{xy}	-5.83	G'_{xy}	0.14	A_{xy}	-5.86	$A_{y,xx}$	0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.01	$A_{z,xx}$	-11.27
g_{yx}	-5.83	G'_{yx}	1.48	A_{yx}	3.33	$A_{x,yy}$	-0.02
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.01	$A_{y,yy}$	0.00
g_{yz}	0.01	G'_{yz}	-0.00	A_{yz}	0.00	$A_{z,yy}$	-9.45
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	-0.00	$A_{x,zz}$	0.01
g_{zy}	0.01	G'_{zy}	-0.00	A_{zy}	0.01	$A_{y,zz}$	-0.00
g_{zz}	-0.00	G'_{zz}	-0.00	A_{zz}	0.00	$A_{z,zz}$	18.22
						$A_{x,xy}, A_{x,yx}$	-0.00
						$A_{y,xy}, A_{y,yx}$	-0.03
						$A_{z,xy}, A_{z,yx}$	-0.01
						$A_{x,xz}, A_{x,zx}$	-14.61
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	0.01
						$A_{x,yz}, A_{x,zy}$	-0.00
						$A_{y,yz}, A_{y,zy}$	-15.31

			$A_{z,yz}, A_{z,zy}$	0.01
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*S51. Sum-Over-All-State Gyration Tensors for 6 Using 6-311+G**:*

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	-1.57
g_{xy}	-64.03	G'_{xy}	0.15	A_{xy}	-3.62	$A_{y,xx}$	0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.02	$A_{z,xx}$	-6.99
g_{yx}	-64.03	G'_{yx}	18.47	A_{yx}	11.59	$A_{x,yy}$	0.73
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.01	$A_{y,yy}$	-0.02
g_{yz}	0.27	G'_{yz}	-0.13	A_{yz}	-0.96	$A_{z,yy}$	18.90
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	-0.00	$A_{x,zz}$	1.30
g_{zy}	0.27	G'_{zy}	0.03	A_{zy}	0.23	$A_{y,zz}$	0.01
g_{zz}	-0.00	G'_{zz}	-0.00	A_{zz}	0.00	$A_{z,zz}$	-16.43
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.51
						$A_{z,xy}, A_{z,yx}$	-0.01
						$A_{x,xz}, A_{x,zx}$	-18.58
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	0.34
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	15.27
						$A_{z,yz}, A_{z,zy}$	-0.01

S52. Sum-Over-All-State Gyration Tensors for 6 Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	-0.01	$A_{x,xx}$	-1.71
g_{xy}	-59.64	G'_{xy}	0.02	A_{xy}	-4.36	$A_{y,xx}$	-0.00
g_{xz}	0.00	G'_{xz}	-0.00	A_{xz}	-0.00	$A_{z,xx}$	-7.21
g_{yx}	-59.64	G'_{yx}	17.16	A_{yx}	4.37	$A_{x,yy}$	0.59
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.00	$A_{y,yy}$	-0.02
g_{yz}	0.20	G'_{yz}	-0.11	A_{yz}	-0.92	$A_{z,yy}$	12.53
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	0.01	$A_{x,zz}$	0.62
g_{zy}	0.20	G'_{zy}	0.04	A_{zy}	0.24	$A_{y,zz}$	0.01
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.01	$A_{z,zz}$	2.68
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.35
						$A_{z,xy}, A_{z,yx}$	0.02
						$A_{x,xz}, A_{x,zx}$	-11.58
						$A_{y,xz}, A_{y,zx}$	0.01
						$A_{z,xz}, A_{z,zx}$	-0.30
						$A_{x,yz}, A_{x,zy}$	0.02
						$A_{y,yz}, A_{y,zy}$	8.17

			$A_{z,yz}, A_{z,zy}$	0.01
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*S53. Sum-Over-All-State Gyration Tensors for 7 Using 6-311+G**:*

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	-0.00	$A_{x,xx}$	0.01
g_{xy}	-10.47	G'_{xy}	-0.03	A_{xy}	-12.06	$A_{y,xx}$	-0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.01	$A_{z,xx}$	3.74
g_{yx}	-10.47	G'_{yx}	2.80	A_{yx}	2.04	$A_{x,yy}$	0.01
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.00	$A_{y,yy}$	0.00
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.00	$A_{z,yy}$	6.71
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	-0.02
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	0.00	$A_{y,zz}$	0.00
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.00	$A_{z,zz}$	-99.33
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	1.69
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	-0.02
						$A_{x,yz}, A_{x,zy}$	-0.00
						$A_{y,yz}, A_{y,zy}$	-5.34
						$A_{z,yz}, A_{z,zy}$	-0.00

S54. Sum-Over-All-State Gyration Tensors for 7 Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	0.00
g_{xy}	-9.81	G'_{xy}	0.08	A_{xy}	-20.27	$A_{y,xx}$	-0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.00	$A_{z,xx}$	1.95
g_{yx}	-9.81	G'_{yx}	2.38	A_{yx}	5.31	$A_{x,yy}$	0.00
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	-0.01	$A_{y,yy}$	0.00
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.01	$A_{z,yy}$	14.71
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	-0.01
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	0.01	$A_{y,zz}$	-0.01
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.00	$A_{z,zz}$	-100.65
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-0.00
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-3.36
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	-0.03
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	-5.56

			$A_{z,vz}, A_{z,zv}$	-0.01
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S55. Sum-Over-All-State Gyration Tensors for 8 Using 6-311+G:**

$g_{a\beta}$		$G'_{a\beta}$		$A_{a\beta}$		$A_{a,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	-0.00	A_{xx}	-0.01	$A_{x,xx}$	0.02
g_{xy}	-73.20	G'_{xy}	0.38	A_{xy}	-48.06	$A_{y,xx}$	0.00
g_{xz}	0.01	G'_{xz}	0.00	A_{xz}	0.05	$A_{z,xx}$	-4.13
g_{yx}	-73.20	G'_{yx}	19.77	A_{yx}	9.39	$A_{x,yy}$	-0.17
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.01	$A_{y,yy}$	-0.03
g_{yz}	0.03	G'_{yz}	-0.01	A_{yz}	-0.08	$A_{z,yy}$	111.90
g_{zx}	0.01	G'_{zx}	-0.00	A_{zx}	0.00	$A_{x,zz}$	0.32
g_{zy}	0.03	G'_{zy}	-0.01	A_{zy}	-0.07	$A_{y,zz}$	0.08
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	-0.01	$A_{z,zz}$	-300.15
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-0.10
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	-13.52
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	0.24
						$A_{x,yz}, A_{x,zy}$	-0.01
						$A_{y,yz}, A_{y,zy}$	63.84
						$A_{z,yz}, A_{z,zy}$	0.03

S56. Sum-Over-All-State Gyration Tensors for 8 Using aug-cc-pVDZ:

$g_{a\beta}$		$G'_{a\beta}$		$A_{a\beta}$		$A_{a,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	-0.02	$A_{x,xx}$	0.03
g_{xy}	-63.59	G'_{xy}	0.49	A_{xy}	-60.55	$A_{y,xx}$	-0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.03	$A_{z,xx}$	-7.34
g_{yx}	-63.59	G'_{yx}	16.63	A_{yx}	10.95	$A_{x,yy}$	-0.12
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.00	$A_{y,yy}$	-0.01
g_{yz}	0.04	G'_{yz}	-0.01	A_{yz}	0.01	$A_{z,yy}$	114.69
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	0.25
g_{zy}	0.04	G'_{zy}	-0.01	A_{zy}	-0.01	$A_{y,zz}$	-0.00
g_{zz}	0.01	G'_{zz}	0.00	A_{zz}	0.02	$A_{z,zz}$	-279.95
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-0.11
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	-18.29
						$A_{y,xz}, A_{y,zx}$	-0.02
						$A_{z,xz}, A_{z,zx}$	0.26
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	54.15

			$A_{z,yz}, A_{z,zy}$	0.02
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S57. Sum-Over-All-State Gyration Tensors for 9 Using 6-311+G:**

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	-0.00	A_{xx}	-0.00	$A_{x,xx}$	0.00
g_{xy}	-9.04	G'_{xy}	0.27	A_{xy}	38.82	$A_{y,xx}$	0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.03	$A_{z,xx}$	-0.65
g_{yx}	-9.04	G'_{yx}	3.44	A_{yx}	7.53	$A_{x,yy}$	-0.00
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.00	$A_{y,yy}$	0.02
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.00	$A_{z,yy}$	-129.62
g_{zx}	-0.00	G'_{zx}	-0.00	A_{zx}	-0.00	$A_{x,zz}$	0.00
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.00	$A_{y,zz}$	-0.01
g_{zz}	0.00	G'_{zz}	-0.00	A_{zz}	0.00	$A_{z,zz}$	-1.79
						$A_{x,xy}, A_{x,yx}$	-0.00
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-8.18
						$A_{y,xz}, A_{y,zx}$	-0.01
						$A_{z,xz}, A_{z,zx}$	0.00
						$A_{x,yz}, A_{x,zy}$	-0.00
						$A_{y,yz}, A_{y,zy}$	-90.80
						$A_{z,yz}, A_{z,zy}$	0.01

S58. Sum-Over-All-State Gyration Tensors for 9 Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	0.00
g_{xy}	-9.23	G'_{xy}	0.43	A_{xy}	24.10	$A_{y,xx}$	-0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	-0.01	$A_{z,xx}$	-2.69
g_{yx}	-9.23	G'_{yx}	3.13	A_{yx}	13.48	$A_{x,yy}$	-0.00
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.00	$A_{y,yy}$	-0.01
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.00	$A_{z,yy}$	-112.96
g_{zx}	0.00	G'_{zx}	-0.00	A_{zx}	0.00	$A_{x,zz}$	0.00
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.01	$A_{y,zz}$	0.00
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.00	$A_{z,zz}$	-0.36
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-16.17
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	0.00
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	-88.87

			$A_{z,yz}, A_{z,zy}$	0.01
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S59. Sum-Over-All-State Gyration Tensors for **10** Using 6-311+G**.

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	-0.00	$A_{x,xx}$	0.01
g_{xy}	-21.72	G'_{xy}	0.29	A_{xy}	24.20	$A_{y,xx}$	0.01
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	-0.00	$A_{z,xx}$	-10.62
g_{yx}	-21.72	G'_{yx}	6.80	A_{yx}	10.60	$A_{x,yy}$	0.01
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.01	$A_{y,yy}$	0.00
g_{yz}	-0.00	G'_{yz}	-0.00	A_{yz}	-0.01	$A_{z,yy}$	-117.73
g_{zx}	0.00	G'_{zx}	-0.00	A_{zx}	-0.01	$A_{x,zz}$	0.01
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.03	$A_{y,zz}$	0.00
g_{zz}	-0.00	G'_{zz}	0.00	A_{zz}	-0.01	$A_{z,zz}$	29.36
						$A_{x,xy}, A_{x,yx}$	-0.00
						$A_{y,xy}, A_{y,yx}$	0.03
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	-21.22
						$A_{y,xz}, A_{y,zx}$	0.00
						$A_{z,xz}, A_{z,zx}$	-0.01
						$A_{x,yz}, A_{x,zy}$	-0.00
						$A_{y,yz}, A_{y,zy}$	-93.53
						$A_{z,yz}, A_{z,zy}$	0.00

S60. Sum-Over-All-State Gyration Tensors for **10** Using aug-cc-pVDZ:

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	0.00
g_{xy}	-23.66	G'_{xy}	0.29	A_{xy}	4.71	$A_{y,xx}$	-0.01
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	-0.00	$A_{z,xx}$	-13.09
g_{yx}	-23.66	G'_{yx}	6.80	A_{yx}	6.95	$A_{x,yy}$	-0.02
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	-0.00	$A_{y,yy}$	-0.02
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.01	$A_{z,yy}$	-103.75
g_{zx}	0.00	G'_{zx}	-0.00	A_{zx}	0.01	$A_{x,zz}$	0.00
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.05	$A_{y,zz}$	0.00
g_{zz}	-0.00	G'_{zz}	0.00	A_{zz}	-0.00	$A_{z,zz}$	30.48
						$A_{x,xy}, A_{x,yx}$	0.01
						$A_{y,xy}, A_{y,yx}$	0.03
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	-20.04
						$A_{y,xz}, A_{y,zx}$	0.00
						$A_{z,xz}, A_{z,zx}$	-0.00
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	-99.04

			$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.01
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S61. Sum-Over-All-State Gyration Tensors for **11** Using 6-311+G**.

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.02	$\mathbf{G}'_{xx}$	-0.00	$\mathbf{A}_{xx}$	-0.10	$\mathbf{A}_{x,xx}$	-0.00
$\mathbf{g}_{xy}$	-86.24	$\mathbf{G}'_{xy}$	0.08	$\mathbf{A}_{xy}$	-205.86	$\mathbf{A}_{y,xx}$	-0.01
$\mathbf{g}_{xz}$	-0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	-0.00	$\mathbf{A}_{z,xx}$	1.83
$\mathbf{g}_{yx}$	-86.24	$\mathbf{G}'_{yx}$	19.91	$\mathbf{A}_{yx}$	4.08	$\mathbf{A}_{x,yy}$	-0.01
$\mathbf{g}_{yy}$	-0.02	$\mathbf{G}'_{yy}$	0.01	$\mathbf{A}_{yy}$	0.08	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.01	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	-0.01	$\mathbf{A}_{z,yy}$	-121.44
$\mathbf{g}_{zx}$	-0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.01	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	-0.01	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.02	$\mathbf{A}_{y,zz}$	0.01
$\mathbf{g}_{zz}$	0.04	$\mathbf{G}'_{zz}$	-0.00	$\mathbf{A}_{zz}$	0.02	$\mathbf{A}_{z,zz}$	6.83
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	-0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.01
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	-0.15
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-2.25
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	-0.25
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	-0.01
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	-0.22
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-327.30
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.01

S62. Sum-Over-All-State Gyration Tensors for **11** Using aug-cc-pVDZ:

$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.02	$\mathbf{G}'_{xx}$	-0.00	$\mathbf{A}_{xx}$	-0.04	$\mathbf{A}_{x,xx}$	-0.01
$\mathbf{g}_{xy}$	-78.45	$\mathbf{G}'_{xy}$	0.28	$\mathbf{A}_{xy}$	-193.27	$\mathbf{A}_{y,xx}$	-0.01
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	-0.01	$\mathbf{A}_{z,xx}$	-0.54
$\mathbf{g}_{yx}$	-78.45	$\mathbf{G}'_{yx}$	17.92	$\mathbf{A}_{yx}$	10.78	$\mathbf{A}_{x,yy}$	-0.00
$\mathbf{g}_{yy}$	-0.03	$\mathbf{G}'_{yy}$	0.01	$\mathbf{A}_{yy}$	0.02	$\mathbf{A}_{y,yy}$	0.01
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	-0.01	$\mathbf{A}_{z,yy}$	-97.16
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.01	$\mathbf{A}_{x,zz}$	-0.01
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.01	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.04	$\mathbf{G}'_{zz}$	-0.00	$\mathbf{A}_{zz}$	0.02	$\mathbf{A}_{z,zz}$	6.49
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.01
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	-0.14
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-11.32
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	-0.18
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	-0.02
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	-0.16
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-290.43

			$A_{z,yz}, A_{z,zv}$	0.01
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S63. Sum-Over-All-State Gyration Tensors for 12 Using 6-311+G.**

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.43	G'_{xx} -0.42	A_{xx} 5.50	$A_{x,xx}$ 2.86
g_{xy} -195.25	G'_{xy} 0.14	A_{xy} -283.45	$A_{y,xx}$ -1.63
g_{xz} -3.40	G'_{xz} -0.25	A_{xz} 21.28	$A_{z,xx}$ -5.31
g_{yx} -195.25	G'_{yx} 49.50	A_{yx} 9.10	$A_{x,yy}$ -0.18
g_{yy} -3.11	G'_{yy} -0.12	A_{yy} -3.29	$A_{y,yy}$ -74.64
g_{yz} -0.57	G'_{yz} 0.08	A_{yz} 2.03	$A_{z,yy}$ -324.49
g_{zx} -3.40	G'_{zx} 1.53	A_{zx} -8.63	$A_{x,zz}$ -1.84
g_{zy} -0.57	G'_{zy} 0.00	A_{zy} -5.24	$A_{y,zz}$ -21.24
g_{zz} -0.85	G'_{zz} 0.05	A_{zz} -2.21	$A_{z,zz}$ 126.15
			$A_{x,xy}, A_{x,yx}$ -10.25
			$A_{y,xy}, A_{y,yx}$ 5.06
			$A_{z,xy}, A_{z,yx}$ 5.97
			$A_{x,xz}, A_{x,zx}$ -14.41
			$A_{y,xz}, A_{y,zx}$ 11.47
			$A_{z,xz}, A_{z,zx}$ 0.20
			$A_{x,yz}, A_{x,zy}$ 9.26
			$A_{y,yz}, A_{y,zy}$ -607.94
			$A_{z,yz}, A_{z,zy}$ -42.52

S64. Sum-Over-All-State Gyration Tensors for 12 Using aug-cc-pVDZ.

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.31	G'_{xx} -0.44	A_{xx} 4.80	$A_{x,xx}$ 2.96
g_{xy} -189.01	G'_{xy} 0.15	A_{xy} -278.63	$A_{y,xx}$ -1.45
g_{xz} -3.54	G'_{xz} -0.27	A_{xz} 22.36	$A_{z,xx}$ -9.53
g_{yx} -189.01	G'_{yx} 47.70	A_{yx} 4.80	$A_{x,yy}$ -0.42
g_{yy} -3.30	G'_{yy} -0.11	A_{yy} -3.29	$A_{y,yy}$ -72.54
g_{yz} -0.49	G'_{yz} 0.08	A_{yz} 2.44	$A_{z,yy}$ -306.19
g_{zx} -3.54	G'_{zx} 1.60	A_{zx} -9.40	$A_{x,zz}$ -2.15
g_{zy} -0.49	G'_{zy} -0.00	A_{zy} -5.06	$A_{y,zz}$ -20.11
g_{zz} -0.74	G'_{zz} 0.04	A_{zz} -1.51	$A_{z,zz}$ 136.14
			$A_{x,xy}, A_{x,yx}$ -10.85
			$A_{y,xy}, A_{y,yx}$ 4.64
			$A_{z,xy}, A_{z,yx}$ 5.33
			$A_{x,xz}, A_{x,zx}$ -14.33
			$A_{y,xz}, A_{y,zx}$ 10.12
			$A_{z,xz}, A_{z,zx}$ 0.28
			$A_{x,yz}, A_{x,zy}$ 8.61
			$A_{y,yz}, A_{y,zy}$ -584.82

			$A_{z,vz}, A_{z,vz}$	-42.47
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S65. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **1** Using 6-311+G**.

Excited States Included: 1, 5, 11, 34

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -18.76	G'_{xy} 0.00	A_{xy} -41.72	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -23.11
g_{yx} -18.76	G'_{yx} 3.85	A_{yx} -23.11	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ -0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -44.68
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} -0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 5.98
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -86.40
			$A_{z,yz}, A_{z,zy}$ 0.00

S66. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **1** Using aug-cc-pVDZ:

Excited States Included: 1, 5, 13, 40

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -19.25	G'_{xy} 0.00	A_{xy} -44.36	$A_{y,xx}$ -0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -23.51
g_{yx} -19.25	G'_{yx} 3.91	A_{yx} -23.51	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -38.99
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 6.16
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -83.35
			$A_{z,yz}, A_{z,zy}$ 0.00

			A_{zVZ}, A_{zZV}	0.00
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S67. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 2 Using 6-311+G.**

Excited States Included: 1, 8, 18, 46

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} -0.00	G'_{xx} 0.00	A_{xx} -0.01	$A_{x,xx}$ 0.00
g_{xy} -15.85	G'_{xy} 0.00	A_{xy} -95.03	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -1.18
g_{yx} -15.85	G'_{yx} 2.26	A_{yx} -1.18	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.01	$A_{y,yy}$ 0.00
g_{yz} -0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -73.87
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} -0.00	G'_{zy} 0.00	A_{zy} -0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 5.34
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.01
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -168.90
			$A_{z,yz}, A_{z,zy}$ 0.00

S68. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 2 Using aug-cc-pVDZ:

Excited States Included: 1, 11, 24, 98

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -21.01	G'_{xy} -0.00	A_{xy} -161.97	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ 0.08
g_{yx} -21.01	G'_{yx} 2.17	A_{yx} 0.35	$A_{x,yy}$ -0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} -0.00	A_{yz} -0.00	$A_{z,yy}$ 0.71
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.02	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 0.08
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.02
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -0.27
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ -0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -161.25

			$A_{z,vz}, A_{z,zv}$	0.00
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S69. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **3** Using 6-311+G**:

Excited States Included: 1, 3, 5, 7, 9, 14, 16, 21, 30, 32, 42, 52, 60, 68, 81, 98, 105, 127, 144, 155, 164, 213, 234, 315, 382

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -148.23	G'_{xy} 0.00	A_{xy} -227.74	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -22.89
g_{yx} -148.23	G'_{yx} 36.66	A_{yx} -22.89	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -4.29
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -86.35
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -232.03
			$A_{z,yz}, A_{z,zy}$ 0.00

S70. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **3** Using aug-cc-pVDZ:

Excited States Included: 1, 3, 5, 7, 11, 17, 18, 25, 32, 37, 49, 60, 65, 78, 91, 110, 123, 158, 168, 198, 211, 254, 269, 356, 457

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -141.91	G'_{xy} 0.00	A_{xy} -186.10	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -12.59
g_{yx} -141.91	G'_{yx} 36.09	A_{yx} -12.59	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -33.91
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -70.25
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -220.01
			$A_{z,yz}, A_{z,zy}$ 0.00

			$A_{z,vz}, A_{z,zv}$	0.00
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S71. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 4 Using 6-311+G:**

Excited States Included: 1, 2, 5, 8, 10, 13, 15, 25, 26, 34, 37, 43, 57, 64, 70, 86, 108, 132, 138, 170, 176, 269, 372, 464, 546

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -166.88	G'_{xy} 0.00	A_{xy} -209.30	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -8.58
g_{yx} -166.88	G'_{yx} 42.82	A_{yx} -8.58	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -539.87
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} -0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -114.61
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.0
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -749.18
			$A_{z,yz}, A_{z,zv}$ 0.00

S72. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 4 Using aug-cc-pVDZ:

Excited States Included: 1, 2, 7, 8, 12, 14, 17, 27, 30, 39, 40, 45, 49, 64, 79, 92, 101, 103, 127, 164, 167, 178, 222, 268, 327

$g_{a\beta}$	$G'_{a\beta}$	$A_{a\beta}$	$A_{a,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -171.03	G'_{xy} 0.00	A_{xy} -259.34	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -4.37
g_{yx} -171.03	G'_{yx} 42.92	A_{yx} -4.37	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -521.41
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ -124.99
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zv}$ -780.75

			A_{zVZ}, A_{zZV}	0.00
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S73. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 5 Using 6-311+G.**

Excited States Included: 1, 5, 13, 28

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.01	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	0.04
g_{xy}	-8.01	G'_{xy}	0.00	A_{xy}	9.93	$A_{y,xx}$	0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.00	$A_{z,xx}$	-24.02
g_{yx}	-8.01	G'_{yx}	1.97	A_{yx}	-24.02	$A_{x,yy}$	0.06
g_{yy}	-0.01	G'_{yy}	0.00	A_{yy}	0.00	$A_{y,yy}$	-0.01
g_{yz}	-0.07	G'_{yz}	-0.00	A_{yz}	-0.41	$A_{z,yy}$	-30.55
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	-0.03
g_{zy}	-0.07	G'_{zy}	0.02	A_{zy}	0.14	$A_{y,zz}$	0.01
g_{zz}	-0.01	G'_{zz}	-0.00	A_{zz}	-0.00	$A_{z,zz}$	15.41
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-0.08
						$A_{z,xy}, A_{z,yx}$	-0.01
						$A_{x,xz}, A_{x,zx}$	0.00
						$A_{y,xz}, A_{y,zx}$	-0.01
						$A_{z,xz}, A_{z,zx}$	-0.44
						$A_{x,yz}, A_{x,zy}$	-0.01
						$A_{y,yz}, A_{y,zy}$	-20.62
						$A_{z,yz}, A_{z,zy}$	0.00

S74. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 5 Using aug-cc-pVDZ:

Excited States Included: 1, 8, 17, 37

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.01	G'_{xx}	-0.00	A_{xx}	0.07	$A_{x,xx}$	0.00
g_{xy}	-4.82	G'_{xy}	0.00	A_{xy}	-17.36	$A_{y,xx}$	0.00
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.00	$A_{z,xx}$	29.81
g_{yx}	-4.82	G'_{yx}	1.69	A_{yx}	29.81	$A_{x,yy}$	0.00
g_{yy}	-0.01	G'_{yy}	-0.00	A_{yy}	-0.08	$A_{y,yy}$	0.00
g_{yz}	0.04	G'_{yz}	-0.08	A_{yz}	0.02	$A_{z,yy}$	3.13
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	0.00
g_{zy}	0.04	G'_{zy}	-0.00	A_{zy}	0.20	$A_{y,zz}$	-0.00
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.01	$A_{z,zz}$	3.84
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-0.20
						$A_{z,xy}, A_{z,yx}$	-0.06
						$A_{x,xz}, A_{x,zx}$	0.00
						$A_{y,xz}, A_{y,zx}$	0.01
						$A_{z,xz}, A_{z,zx}$	0.02
						$A_{x,yz}, A_{x,zy}$	0.02
						$A_{y,yz}, A_{y,zy}$	-14.23

			$A_{z,vz}, A_{z,zv}$	0.00
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S75. Sum-Over- $\pi \rightarrow \pi^$ State Gyration Tensors for 6 Using 6-311+G**.*

Excited States Included: 1, 3, 12, 16, 24, 37, 48, 72, 115

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.03	G'_{xx} 0.00	A_{xx} -0.19	$A_{x,xx}$ 0.00
g_{xy} -67.82	G'_{xy} -0.00	A_{xy} -8.71	$A_{y,xx}$ 0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.02	$A_{z,xx}$ -5.87
g_{yx} -67.82	G'_{yx} 19.18	A_{yx} -5.96	$A_{x,yy}$ -0.41
g_{yy} 0.03	G'_{yy} 0.01	A_{yy} 0.10	$A_{y,yy}$ -0.00
g_{yz} -0.13	G'_{yz} -0.10	A_{yz} -2.19	$A_{z,yy}$ 14.70
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} -0.00	$A_{x,zz}$ 0.54
g_{zy} -0.13	G'_{zy} 0.07	A_{zy} -0.70	$A_{y,zz}$ 0.02
g_{zz} 0.08	G'_{zz} 0.00	A_{zz} 0.09	$A_{z,zz}$ -15.61
			$A_{x,xy}, A_{x,yx}$ -0.00
			$A_{y,xy}, A_{y,yx}$ 0.29
			$A_{z,xy}, A_{z,yx}$ 0.06
			$A_{x,xz}, A_{x,zx}$ 0.09
			$A_{y,xz}, A_{y,zx}$ -0.13
			$A_{z,xz}, A_{z,zx}$ -1.66
			$A_{x,yz}, A_{x,zy}$ -0.04
			$A_{y,yz}, A_{y,zy}$ 5.99
			$A_{z,vz}, A_{z,zv}$ -0.00

S76. Sum-Over- $\pi \rightarrow \pi^$ State Gyration Tensors for 6 Using aug-cc-pVDZ:*

Excited States Included: 1, 5, 13, 17, 29, 42, 75, 84, 142

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} -0.00	G'_{xx} 0.00	A_{xx} 0.01	$A_{x,xx}$ 0.91
g_{xy} -64.95	G'_{xy} -0.01	A_{xy} -12.89	$A_{y,xx}$ -0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.02	$A_{z,xx}$ -3.98
g_{yx} -64.95	G'_{yx} 18.31	A_{yx} -4.06	$A_{x,yy}$ 4.37
g_{yy} -0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.00
g_{yz} 0.16	G'_{yz} -0.21	A_{yz} -1.51	$A_{z,yy}$ 4.77
g_{zx} 0.00	G'_{zx} -0.00	A_{zx} 0.00	$A_{x,zz}$ -3.50
g_{zy} 0.16	G'_{zy} 0.26	A_{zy} 5.38	$A_{y,zz}$ -0.00
g_{zz} -0.00	G'_{zz} -0.00	A_{zz} -0.01	$A_{z,zz}$ -5.14
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -1.01
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.08
			$A_{y,xz}, A_{y,zx}$ 0.01
			$A_{z,xz}, A_{z,zx}$ -5.01
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,vz}, A_{y,zv}$ -8.12

			$A_{z,vz}, A_{z,zv}$	-0.02
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S77. Sum-Over- $\pi \rightarrow \pi^$ State Gyration Tensors for 7 Using 6-311+G**.*

Excited States Included: 1, 2, 12, 25, 26, 31, 49, 79, 140

$g_{a\beta}$		$G'_{a\beta}$		$A_{a\beta}$		$A_{a,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	0.14
g_{xy}	-9.09	G'_{xy}	0.00	A_{xy}	-28.91	$A_{y,xx}$	-0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.00	$A_{z,xx}$	16.45
g_{yx}	-9.09	G'_{yx}	2.32	A_{yx}	16.45	$A_{x,yy}$	0.12
g_{yy}	-0.00	G'_{yy}	0.00	A_{yy}	-0.01	$A_{y,yy}$	0.00
g_{yz}	0.06	G'_{yz}	0.00	A_{yz}	0.67	$A_{z,yy}$	34.35
g_{zx}	0.00	G'_{zx}	0.00	A_{zx}	0.00	$A_{x,zz}$	-0.69
g_{zy}	0.06	G'_{zy}	0.00	A_{zy}	0.11	$A_{y,zz}$	-0.00
g_{zz}	-0.00	G'_{zz}	-0.00	A_{zz}	0.00	$A_{z,zz}$	-117.41
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	-0.01
						$A_{x,xz}, A_{x,zx}$	-0.00
						$A_{y,xz}, A_{y,zx}$	-0.00
						$A_{z,xz}, A_{z,zx}$	-0.02
						$A_{x,yz}, A_{x,zy}$	0.00
						$A_{y,yz}, A_{y,zy}$	5.44
						$A_{z,vz}, A_{z,zv}$	-0.00

S78. Sum-Over- $\pi \rightarrow \pi^$ State Gyration Tensors for 7 Using aug-cc-pVDZ:*

Excited States Included: 1, 2, 15, 17, 26, 28, 34, 94, 114

$g_{a\beta}$		$G'_{a\beta}$		$A_{a\beta}$		$A_{a,\beta\gamma}$	
g_{xx}	-0.02	G'_{xx}	0.00	A_{xx}	0.19	$A_{x,xx}$	-0.00
g_{xy}	-8.48	G'_{xy}	0.00	A_{xy}	-38.04	$A_{y,xx}$	-0.01
g_{xz}	-0.00	G'_{xz}	0.00	A_{xz}	-0.01	$A_{z,xx}$	18.23
g_{yx}	-8.48	G'_{yx}	1.97	A_{yx}	18.23	$A_{x,yy}$	0.00
g_{yy}	0.00	G'_{yy}	-0.01	A_{yy}	0.01	$A_{y,yy}$	0.00
g_{yz}	-0.00	G'_{yz}	0.00	A_{yz}	-0.01	$A_{z,yy}$	31.50
g_{zx}	-0.00	G'_{zx}	0.00	A_{zx}	0.01	$A_{x,zz}$	0.00
g_{zy}	-0.00	G'_{zy}	0.00	A_{zy}	-0.00	$A_{y,zz}$	-0.01
g_{zz}	-0.09	G'_{zz}	0.00	A_{zz}	-0.20	$A_{z,zz}$	-112.10
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.00
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	-0.00
						$A_{y,xz}, A_{y,zx}$	0.19
						$A_{z,xz}, A_{z,zx}$	-0.01
						$A_{x,yz}, A_{x,zy}$	-0.01
						$A_{y,vz}, A_{y,zv}$	-6.54

			A_{zVZ}, A_{zZV}	0.00
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S79. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **8** Using 6-311+G**:

Excited States Included: 1, 2, 6, 9, 13, 20, 23, 35, 39, 45, 87, 93, 134, 163, 181, 258

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	-0.00	G'_{xx}	-0.00	A_{xx}	-0.03	$A_{x,xx}$	-0.08
g_{xy}	-79.94	G'_{xy}	-0.00	A_{xy}	-93.99	$A_{y,xx}$	0.00
g_{xz}	0.00	G'_{xz}	0.00	A_{xz}	0.02	$A_{z,xx}$	-17.41
g_{yx}	-79.94	G'_{yx}	20.34	A_{yx}	-17.41	$A_{x,yy}$	-0.10
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	0.01	$A_{y,yy}$	-0.01
g_{yz}	-0.04	G'_{yz}	0.01	A_{yz}	-0.10	$A_{z,yy}$	118.10
g_{zx}	0.00	G'_{zx}	-0.00	A_{zx}	-0.00	$A_{x,zz}$	0.31
g_{zy}	-0.04	G'_{zy}	0.00	A_{zy}	-0.19	$A_{y,zz}$	0.06
g_{zz}	0.01	G'_{zz}	0.00	A_{zz}	0.02	$A_{z,zz}$	-299.13
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	0.09
						$A_{z,xy}, A_{z,yx}$	0.00
						$A_{x,xz}, A_{x,zx}$	0.00
						$A_{y,xz}, A_{y,zx}$	-0.03
						$A_{z,xz}, A_{z,zx}$	0.22
						$A_{x,yz}, A_{x,zy}$	-0.01
						$A_{y,yz}, A_{y,zy}$	24.11
						$A_{z,yz}, A_{z,zy}$	0.04

S80. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **8** Using aug-cc-pVDZ:

Excited States Included: 1, 2, 8, 9, 15, 21, 27, 38, 49, 58, 98, 122, 160, 181, 219, 309

$g_{\alpha\beta}$		$G'_{\alpha\beta}$		$A_{\alpha\beta}$		$A_{\alpha,\beta\gamma}$	
g_{xx}	0.00	G'_{xx}	0.00	A_{xx}	0.00	$A_{x,xx}$	-0.03
g_{xy}	-67.00	G'_{xy}	0.00	A_{xy}	-66.66	$A_{y,xx}$	0.01
g_{xz}	-0.01	G'_{xz}	0.00	A_{xz}	-0.05	$A_{z,xx}$	-18.51
g_{yx}	-67.00	G'_{yx}	17.25	A_{yx}	-18.51	$A_{x,yy}$	-0.05
g_{yy}	0.00	G'_{yy}	0.00	A_{yy}	-0.02	$A_{y,yy}$	-0.00
g_{yz}	0.58	G'_{yz}	-0.10	A_{yz}	0.21	$A_{z,yy}$	121.08
g_{zx}	-0.01	G'_{zx}	0.00	A_{zx}	-0.01	$A_{x,zz}$	-0.06
g_{zy}	0.58	G'_{zy}	-0.00	A_{zy}	2.37	$A_{y,zz}$	-0.01
g_{zz}	0.00	G'_{zz}	0.00	A_{zz}	0.02	$A_{z,zz}$	-300.32
						$A_{x,xy}, A_{x,yx}$	0.00
						$A_{y,xy}, A_{y,yx}$	-2.43
						$A_{z,xy}, A_{z,yx}$	-0.00
						$A_{x,xz}, A_{x,zx}$	0.00
						$A_{y,xz}, A_{y,zx}$	0.00
						$A_{z,xz}, A_{z,zx}$	0.14
						$A_{x,yz}, A_{x,zy}$	0.02
						$A_{y,yz}, A_{y,zy}$	54.42

			$A_{z,vz}, A_{z,zv}$	0.04
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S81. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **9** Using 6-311+G**.

Excited States Included: 1, 2, 3, 5, 32, 39, 63, 79, 173

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.01	$A_{x,xx}$ 0.00
g_{xy} -11.16	G'_{xy} 0.00	A_{xy} 23.50	$A_{y,xx}$ 0.00
g_{xz} -0.00	G'_{xz} 0.00	A_{xz} -0.02	$A_{z,xx}$ -0.74
g_{yx} -11.16	G'_{yx} 3.76	A_{yx} -0.74	$A_{x,yy}$ 0.00
g_{yy} -0.00	G'_{yy} -0.00	A_{yy} -0.00	$A_{y,yy}$ 0.02
g_{yz} 0.00	G'_{yz} 0.00	A_{yz} 0.00	$A_{z,yy}$ -109.45
g_{zx} -0.00	G'_{zx} -0.00	A_{zx} -0.00	$A_{x,zz}$ 0.00
g_{zy} 0.00	G'_{zy} 0.00	A_{zy} 0.00	$A_{y,zz}$ -0.00
g_{zz} -0.00	G'_{zz} 0.00	A_{zz} -0.01	$A_{z,zz}$ 11.97
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.00
			$A_{z,xy}, A_{z,yx}$ -0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.01
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -85.95
			$A_{z,yz}, A_{z,zy}$ 0.01

S82. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **9** Using aug-cc-pVDZ:

Excited States Included: 1, 2, 4, 7, 36, 47, 79, 88, 219

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -11.11	G'_{xy} 0.00	A_{xy} 26.81	$A_{y,xx}$ -0.00
g_{xz} -0.00	G'_{xz} 0.00	A_{xz} -0.01	$A_{z,xx}$ -2.80
g_{yx} -11.11	G'_{yx} 3.77	A_{yx} -2.80	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} -0.02	$A_{y,yy}$ -0.01
g_{yz} 0.01	G'_{yz} -0.00	A_{yz} 0.00	$A_{z,yy}$ -109.13
g_{zx} -0.00	G'_{zx} -0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} 0.01	G'_{zy} 0.00	A_{zy} 0.03	$A_{y,zz}$ -0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.02	$A_{z,zz}$ 11.71
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.03
			$A_{z,xy}, A_{z,yx}$ -0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ -0.00
			$A_{z,xz}, A_{z,zx}$ 0.00
			$A_{x,yz}, A_{x,zy}$ 0.02
			$A_{y,yz}, A_{y,zy}$ -82.32

			A_{zVZ}, A_{zZV}	0.01
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S83. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **10** Using 6-311+G**.

Excited States Included: 1, 2, 6, 9, 14, 17, 27, 38, 59

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} -0.00	$A_{x,xx}$ 0.00
g_{xy} -27.18	G'_{xy} 0.00	A_{xy} -7.52	$A_{y,xx}$ 0.00
g_{xz} -0.00	G'_{xz} 0.00	A_{xz} 0.00	$A_{z,xx}$ -4.89
g_{yx} -27.18	G'_{yx} 7.53	A_{yx} -4.89	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ 0.04
g_{yz} -0.00	G'_{yz} -0.00	A_{yz} -0.00	$A_{z,yy}$ -88.10
g_{zx} -0.00	G'_{zx} 0.00	A_{zx} -0.00	$A_{x,zz}$ 0.00
g_{zy} -0.00	G'_{zy} -0.00	A_{zy} -0.03	$A_{y,zz}$ 0.00
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 24.01
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.03
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ -0.00
			$A_{z,xz}, A_{z,zx}$ -0.00
			$A_{x,yz}, A_{x,zy}$ -0.00
			$A_{y,yz}, A_{y,zy}$ -95.62
			$A_{z,yz}, A_{z,zy}$ -0.00

S84. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **10** Using aug-cc-pVDZ:

Excited States Included: 1, 3, 8, 10, 14, 19, 33, 46, 71

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.00	G'_{xx} 0.00	A_{xx} 0.00	$A_{x,xx}$ 0.00
g_{xy} -31.49	G'_{xy} 0.02	A_{xy} -46.20	$A_{y,xx}$ -0.00
g_{xz} 0.00	G'_{xz} 0.00	A_{xz} 0.01	$A_{z,xx}$ -8.38
g_{yx} -31.49	G'_{yx} 7.77	A_{yx} -7.26	$A_{x,yy}$ 0.00
g_{yy} 0.00	G'_{yy} 0.00	A_{yy} 0.00	$A_{y,yy}$ -0.02
g_{yz} -0.00	G'_{yz} 0.00	A_{yz} 0.01	$A_{z,yy}$ -58.65
g_{zx} 0.00	G'_{zx} 0.00	A_{zx} 0.00	$A_{x,zz}$ 0.00
g_{zy} -0.00	G'_{zy} -0.00	A_{zy} -0.05	$A_{y,zz}$ 0.01
g_{zz} 0.00	G'_{zz} 0.00	A_{zz} 0.00	$A_{z,zz}$ 16.08
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ 0.05
			$A_{z,xy}, A_{z,yx}$ 0.00
			$A_{x,xz}, A_{x,zx}$ -1.12
			$A_{y,xz}, A_{y,zx}$ 0.00
			$A_{z,xz}, A_{z,zx}$ 0.01
			$A_{x,yz}, A_{x,zy}$ 0.00
			$A_{y,yz}, A_{y,zy}$ -104.85

			A_{zVZ}, A_{zZV}	0.00
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S85. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **11** Using 6-311+G**.

Excited States Included: 1, 2, 4, 5, 11, 18, 22, 24, 37, 39, 74, 84, 89, 195, 204, 357

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.02	G'_{xx} -0.00	A_{xx} -0.14	$A_{x,xx}$ -0.00
g_{xy} -90.75	G'_{xy} -0.10	A_{xy} -255.69	$A_{y,xx}$ -0.00
g_{xz} -0.00	G'_{xz} 0.00	A_{xz} -0.01	$A_{z,xx}$ -1.99
g_{yx} -90.75	G'_{yx} 20.00	A_{yx} -3.78	$A_{x,yy}$ -0.00
g_{yy} -0.01	G'_{yy} 0.01	A_{yy} 0.04	$A_{y,yy}$ -0.00
g_{yz} 0.02	G'_{yz} -0.00	A_{yz} -0.02	$A_{z,yy}$ -76.52
g_{zx} -0.00	G'_{zx} 0.00	A_{zx} 0.01	$A_{x,zz}$ 0.00
g_{zy} 0.02	G'_{zy} 0.00	A_{zy} 0.15	$A_{y,zz}$ 0.00
g_{zz} 0.06	G'_{zz} -0.00	A_{zz} 0.10	$A_{z,zz}$ 12.59
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.15
			$A_{z,xy}, A_{z,yx}$ -0.11
			$A_{x,xz}, A_{x,zx}$ 1.79
			$A_{y,xz}, A_{y,zx}$ -0.25
			$A_{z,xz}, A_{z,zx}$ -0.01
			$A_{x,yz}, A_{x,zy}$ -0.15
			$A_{y,yz}, A_{y,zy}$ -332.21
			$A_{z,yz}, A_{z,zy}$ 0.01

S86. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for **11** Using aug-cc-pVDZ:

Excited States Included: 1, 2, 6, 7, 12, 23, 27, 28, 47, 50, 87, 96, 123, 225, 234, 415

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.22	G'_{xx} -0.00	A_{xx} 0.46	$A_{x,xx}$ 0.00
g_{xy} -82.09	G'_{xy} -0.00	A_{xy} -197.79	$A_{y,xx}$ -0.01
g_{xz} -0.00	G'_{xz} 0.00	A_{xz} -0.01	$A_{z,xx}$ -0.64
g_{yx} -82.09	G'_{yx} 18.87	A_{yx} -0.64	$A_{x,yy}$ -0.01
g_{yy} 0.04	G'_{yy} 0.01	A_{yy} -0.25	$A_{y,yy}$ -0.00
g_{yz} 0.06	G'_{yz} -0.00	A_{yz} 0.32	$A_{z,yy}$ -81.40
g_{zx} -0.00	G'_{zx} 0.00	A_{zx} 0.01	$A_{x,zz}$ 0.01
g_{zy} 0.06	G'_{zy} -0.01	A_{zy} 0.01	$A_{y,zz}$ -0.00
g_{zz} 0.11	G'_{zz} 0.01	A_{zz} -0.20	$A_{z,zz}$ 5.85
			$A_{x,xy}, A_{x,yx}$ 0.00
			$A_{y,xy}, A_{y,yx}$ -0.02
			$A_{z,xy}, A_{z,yx}$ -0.42
			$A_{x,xz}, A_{x,zx}$ 0.00
			$A_{y,xz}, A_{y,zx}$ 0.04
			$A_{z,xz}, A_{z,zx}$ 0.33
			$A_{x,yz}, A_{x,zy}$ -0.17
			$A_{y,yz}, A_{y,zy}$ -279.19

			$A_{z,vz}, A_{z,zv}$	0.01
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S87. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 12 Using 6-311+G.**

Excited States Included: 1, 2, 6, 7, 12, 14, 15, 21, 28, 45, 47, 52, 64, 71, 116, 135

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.31	G'_{xx} -0.37	A_{xx} 5.57	$A_{x,xx}$ -0.33
g_{xy} -195.00	G'_{xy} 0.02	A_{xy} -250.94	$A_{y,xx}$ -2.36
g_{xz} -3.74	G'_{xz} -0.03	A_{xz} 5.23	$A_{z,xx}$ 15.00
g_{yx} -195.00	G'_{yx} 50.49	A_{yx} 16.15	$A_{x,yy}$ 0.11
g_{yy} -2.78	G'_{yy} -0.11	A_{yy} -1.88	$A_{y,yy}$ -50.30
g_{yz} 0.52	G'_{yz} 0.09	A_{yz} 2.88	$A_{z,yy}$ -325.81
g_{zx} -3.74	G'_{zx} 1.28	A_{zx} 1.92	$A_{x,zz}$ 0.36
g_{zy} 0.52	G'_{zy} -0.19	A_{zy} -0.95	$A_{y,zz}$ -21.31
g_{zz} -1.24	G'_{zz} 0.02	A_{zz} -3.70	$A_{z,zz}$ 111.66
			$A_{x,xy}, A_{x,yx}$ -0.44
			$A_{y,xy}, A_{y,yx}$ 1.06
			$A_{z,xy}, A_{z,yx}$ 4.25
			$A_{x,xz}, A_{x,zx}$ -1.15
			$A_{y,xz}, A_{y,zx}$ 9.82
			$A_{z,xz}, A_{z,zx}$ 3.23
			$A_{x,yz}, A_{x,zy}$ 6.12
			$A_{y,yz}, A_{y,zy}$ -576.75
			$A_{z,yz}, A_{z,zy}$ -26.55

S88. Sum-Over- $\pi \rightarrow \pi^*$ State Gyration Tensors for 12 Using aug-cc-pVDZ:

Excited States Included: 1, 2, 6, 7, 12, 17, 18, 25, 27, 55, 63, 67, 76, 83, 146, 157

$g_{\alpha\beta}$	$G'_{\alpha\beta}$	$A_{\alpha\beta}$	$A_{\alpha,\beta\gamma}$
g_{xx} 0.45	G'_{xx} -0.44	A_{xx} 1.55	$A_{x,xx}$ 0.38
g_{xy} -189.17	G'_{xy} 0.02	A_{xy} -222.26	$A_{y,xx}$ -1.19
g_{xz} -4.04	G'_{xz} -0.03	A_{xz} 6.10	$A_{z,xx}$ 4.80
g_{yx} -189.17	G'_{yx} 49.25	A_{yx} 5.48	$A_{x,yy}$ -0.31
g_{yy} -2.26	G'_{yy} -0.05	A_{yy} 1.24	$A_{y,yy}$ -38.84
g_{yz} -2.42	G'_{yz} 0.00	A_{yz} -13.68	$A_{z,yy}$ -306.29
g_{zx} -4.04	G'_{zx} 1.36	A_{zx} 0.94	$A_{x,zz}$ 3.78
g_{zy} -2.42	G'_{zy} 0.31	A_{zy} -2.45	$A_{y,zz}$ -21.55
g_{zz} -0.28	G'_{zz} 0.08	A_{zz} -2.78	$A_{z,zz}$ 104.66
			$A_{x,xy}, A_{x,yx}$ -0.25
			$A_{y,xy}, A_{y,yx}$ 2.14
			$A_{z,xy}, A_{z,yx}$ 7.04
			$A_{x,xz}, A_{x,zx}$ -0.69
			$A_{y,xz}, A_{y,zx}$ 8.58
			$A_{z,xz}, A_{z,zx}$ -9.90
			$A_{x,yz}, A_{x,zy}$ 5.80
			$A_{y,yz}, A_{y,zy}$ -528.54

			$A_{z,yz}, A_{z,zv}$	-27.65
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S89. Dominant Excited State Data for 1 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 246.03nm

Velocity Oscillator Strength: 0.3166

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r}\nabla + \nabla\mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-0.9687	$(\mathbf{r}\nabla + \nabla\mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2965	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r}\nabla + \nabla\mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r}\nabla + \nabla\mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	842.05
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{yz}$	-0.5185	$\mathbf{R}_{yz}$	0.00
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{zy}$	-0.5185	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r}\nabla + \nabla\mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-20.44	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-85.53	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-20.44	$\mathbf{G}'_{yx}$	3.83	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-85.53
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zv}$	0.00

S90. Dominant Excited State Data for 1 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 247.69nm

Velocity Oscillator Strength: 0.2758

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-1.0029	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2759	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	802.56
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.5107	$\mathbf{R}_{yz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.5107	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-19.80	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-80.18	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-19.80	$\mathbf{G}'_{yx}$	3.78	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-80.18
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S91. Dominant Excited State Data for 2 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 277.11nm

Velocity Oscillator Strength: 0.2348

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-0.4754	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2406	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	692.19
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.8622	$\mathbf{R}_{yz}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.8622	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-22.39	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-173.19	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-22.39	$\mathbf{G}'_{yx}$	2.29	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-173.19
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S92. Dominant Excited State Data for 2 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 279.59nm

Velocity Oscillator Strength: 0.2123

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-0.4616	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2278	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0001	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0001	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0001	$\mathbf{R}_{yx}$	634.42
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.8220	$\mathbf{R}_{yz}$	-0.06
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.8220	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-20.98	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-161.25	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-20.98	$\mathbf{G}'_{yx}$	2.17	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	-0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.02	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	-0.02
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-161.25
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S93. Dominant Excited State Data for 3 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 379.79nm

Velocity Oscillator Strength: 0.3282

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-2.4296	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2430	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	2033.73
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.4098	$\mathbf{R}_{yz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.4098	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-156.08	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-270.32	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-156.08	$\mathbf{G}'_{yx}$	38.45	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-270.32
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S94. Dominant Excited State Data for 3 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 380.88nm

Velocity Oscillator Strength: 0.3310

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-2.3994	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.2437	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	2009.04
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.3895	$\mathbf{R}_{yz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.3895	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-155.58	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-260.74	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-155.58	$\mathbf{G}'_{yx}$	38.54	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-260.74
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S95. Dominant Excited State Data for 4 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 356.18nm

Velocity Oscillator Strength: 0.6132

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-2.3349	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.3430	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	3093.47
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.9278	$\mathbf{R}_{yz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.9278	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-195.57	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-667.36	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-195.57	$\mathbf{G}'_{yx}$	40.30	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-667.36
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S96. Dominant Excited State Data for 4 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 357.49nm

Velocity Oscillator Strength: 0.5970

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-2.3565	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.3378	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	3079.93
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.9296	$\mathbf{R}_{yz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.9296	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-196.81	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-668.09	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-196.81	$\mathbf{G}'_{yx}$	40.63	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-668.09
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S97. Dominant Excited State Data for 5 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 246.30nm

Velocity Oscillator Strength: 0.1002

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-0.9418	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.01
∇_y	0.1667	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0010	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0016	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0010	$\mathbf{R}_{yx}$	392.73
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	-0.0001	$\mathbf{R}_{yy}$	-0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.2907	$\mathbf{R}_{yz}$	-0.83
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.04
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.2907	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0001	$\mathbf{R}_{zz}$	-0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-9.56	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-27.06	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.01	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-9.56	$\mathbf{G}'_{yx}$	2.10	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	-0.01
$\mathbf{g}_{yz}$	0.02	$\mathbf{G}'_{yz}$	-0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.02	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.09	$\mathbf{A}_{y,zz}$	0.01
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	-0.09
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-27.06
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S98. Dominant Excited State Data for 5 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 247.57nm

Velocity Oscillator Strength: 0.0813

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-0.9274	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.002
∇_y	0.1498	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0024	$\mathbf{R}_{xy}$	0.000
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0035	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.000
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0024	$\mathbf{R}_{yx}$	345.688
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.014
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.2735	$\mathbf{R}_{yz}$	-1.699
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.035
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.2735	$\mathbf{R}_{zy}$	0.000
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.000
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-8.52	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-23.28	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-8.52	$\mathbf{G}'_{yx}$	1.89	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.04	$\mathbf{G}'_{yz}$	-0.01	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.04	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.20	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	-0.20
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-23.28
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S99. Dominant Excited State Data for 6 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 411.94nm

Velocity Oscillator Strength: 0.0533

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	2.2547	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.01
∇_y	-0.0940	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0023	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	-0.0136	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0023	$\mathbf{R}_{yx}$	708.35
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	0.1025	$\mathbf{R}_{yz}$	-3.40
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.08
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	0.1025	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.02
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-71.01	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-37.05	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-71.01	$\mathbf{G}'_{yx}$	19.56	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.34	$\mathbf{G}'_{yz}$	-0.12	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.34	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.83	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.83
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-37.05
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S100. Dominant Excited State Data for 6 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 415.13nm

Velocity Oscillator Strength: 0.0435

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	2.2768	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.01
∇_y	-0.0847	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0027	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	-0.0148	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0027	$\mathbf{R}_{yx}$	644.35
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	0.0855	$\mathbf{R}_{yz}$	-3.29
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.08
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	0.0855	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.02
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-66.38	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-28.83	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-66.38	$\mathbf{G}'_{yx}$	18.42	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.34	$\mathbf{G}'_{yz}$	-0.12	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.34	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.91	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.91
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-28.83
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S101. Dominant Excited State Data for 7 Using 6-311+G**:

State Number: 1

Excited State Wavelength: 381.92nm

Velocity Oscillator Strength: 0.0088

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	0.9275	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	-0.0396	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	-0.0001	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	120.08
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.0960	$\mathbf{R}_{yz}$	0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.0960	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-9.38	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-10.56	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-9.38	$\mathbf{G}'_{yx}$	2.45	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-10.56
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S102. Dominant Excited State Data for 7 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 383.18nm

Velocity Oscillator Strength: 0.0068

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	0.9090	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	-0.0348	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	-0.0001	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	104.07
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.0958	$\mathbf{R}_{yz}$	0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.0958	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.00
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-8.21	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-9.34	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-8.21	$\mathbf{G}'_{yx}$	2.14	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-9.39
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S103. Dominant Excited State Data for 8 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 485.59nm

Velocity Oscillator Strength: 0.0147

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	2.0319	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.00
∇_y	-0.0455	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0001	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0005	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0001	$\mathbf{R}_{yx}$	347.46
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	0.0039	$\mathbf{R}_{yz}$	-0.09
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.05
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	0.0039	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0001	$\mathbf{R}_{zz}$	-0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-67.86	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	1.57	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.04	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-67.86	$\mathbf{G}'_{yx}$	19.57	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.02	$\mathbf{G}'_{yz}$	-0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.02	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.04	$\mathbf{A}_{y,zz}$	0.04
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	-0.04
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	1.57
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S104. Dominant Excited State Data for 8 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 488.28nm

Velocity Oscillator Strength: 0.0098

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	2.0653	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.00
∇_y	-0.0370	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0001	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0005	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0001	$\mathbf{R}_{yx}$	286.96
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	0.0201	$\mathbf{R}_{yz}$	-0.07
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.04
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	0.0201	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-57.49	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	6.78	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-57.49	$\mathbf{G}'_{yx}$	16.72	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.02	$\mathbf{G}'_{yz}$	-0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.02	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.03	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	-0.03
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	6.78
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S105. Dominant Excited State Data for 9 Using 6-311+G**:

State Number: 2

Excited State Wavelength: 260.61nm

Velocity Oscillator Strength: 0.0650

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	1.0397	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.00
∇_y	-0.1306	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	249.75
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.0940	$\mathbf{R}_{yz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.0940	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-6.96	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	8.30	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-6.96	$\mathbf{G}'_{yx}$	2.20	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	8.30
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S106. Dominant Excited State Data for 9 Using aug-cc-pVDZ:

State Number: 2

Excited State Wavelength: 261.60nm

Velocity Oscillator Strength: 0.0635

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	1.0614	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.00
∇_y	-0.1288	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	257.49
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	-0.0001	$\mathbf{R}_{yy}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.0763	$\mathbf{R}_{yz}$	-0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.0763	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0001	$\mathbf{R}_{zz}$	-0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-7.24	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	6.73	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	-0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	-0.01	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-7.24	$\mathbf{G}'_{yx}$	2.25	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.01
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	-0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	-0.01
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	6.73
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S107. Dominant Excited State Data for 10 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 277.53nm

Velocity Oscillator Strength: 0.5560

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-1.0347	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.3700	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0001	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0001	$\mathbf{R}_{yx}$	1038.89
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0001	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.2689	$\mathbf{R}_{yz}$	0.09
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.2689	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-33.73	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-83.50	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-33.73	$\mathbf{G}'_{yx}$	7.71	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.03
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.03	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.03
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-83.50
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S108. Dominant Excited State Data for 10 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 279.31nm

Velocity Oscillator Strength: 0.5394nm

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-1.1048	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	0.00
∇_y	0.3633	$(\mathbf{r} \times \nabla)_y$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0001	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0000	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0001	$\mathbf{R}_{yx}$	1101.63
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.2942	$\mathbf{R}_{yz}$	0.08
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0000	$\mathbf{R}_{zx}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.2942	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	0.01
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.00	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	0.00	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-36.35	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-91.72	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-36.35	$\mathbf{G}'_{yx}$	8.26	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.00	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	-0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	-0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	-0.03	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.00	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.00	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.03
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	0.00
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-91.72
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S109. Dominant Excited State Data for 11 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 415.40nm

Velocity Oscillator Strength: 0.1415

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-1.3679	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.14
∇_y	0.1526	$(\mathbf{r} \times \nabla)_y$	-0.0005	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	-0.0003	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	907.31
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.25
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.4769	$\mathbf{R}_{yz}$	0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	-0.0003	$\mathbf{R}_{zx}$	0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.4769	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.51
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.02	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	-0.18	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-93.67	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-290.58	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-93.67	$\mathbf{G}'_{yx}$	20.00	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.01	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.08	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.18	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	-0.18
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-290.58
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S110. Dominant Excited State Data for 11 Using aug-cc-pVDZ:

State Number: 1

Excited State Wavelength: 420.69nm

Velocity Oscillator Strength: 0.1032

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0000	$(\mathbf{r} \times \nabla)_x$	-1.4147	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0000	$\mathbf{R}_{xx}$	-0.12
∇_y	0.1295	$(\mathbf{r} \times \nabla)_y$	-0.0005	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0000	$\mathbf{R}_{xy}$	0.00
∇_z	0.0000	$(\mathbf{r} \times \nabla)_z$	0.0000	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	-0.0002	$\mathbf{R}_{xz}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0000	$\mathbf{R}_{yx}$	791.90
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0000	$\mathbf{R}_{yy}$	-0.26
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.4582	$\mathbf{R}_{yz}$	0.02
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	-0.0002	$\mathbf{R}_{zx}$	0.01
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.4582	$\mathbf{R}_{zy}$	0.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0000	$\mathbf{R}_{zz}$	-0.44
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.03	$\mathbf{G}'_{xx}$	0.00	$\mathbf{A}_{xx}$	-0.11	$\mathbf{A}_{x,xx}$	0.00
$\mathbf{g}_{xy}$	-85.48	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-250.96	$\mathbf{A}_{y,xx}$	0.00
$\mathbf{g}_{xz}$	0.00	$\mathbf{G}'_{xz}$	0.00	$\mathbf{A}_{xz}$	0.00	$\mathbf{A}_{z,xx}$	0.00
$\mathbf{g}_{yx}$	-85.48	$\mathbf{G}'_{yx}$	18.59	$\mathbf{A}_{yx}$	0.00	$\mathbf{A}_{x,yy}$	0.00
$\mathbf{g}_{yy}$	0.00	$\mathbf{G}'_{yy}$	0.01	$\mathbf{A}_{yy}$	0.00	$\mathbf{A}_{y,yy}$	0.00
$\mathbf{g}_{yz}$	0.00	$\mathbf{G}'_{yz}$	0.00	$\mathbf{A}_{yz}$	0.00	$\mathbf{A}_{z,yy}$	0.00
$\mathbf{g}_{zx}$	0.00	$\mathbf{G}'_{zx}$	0.00	$\mathbf{A}_{zx}$	0.00	$\mathbf{A}_{x,zz}$	0.00
$\mathbf{g}_{zy}$	0.00	$\mathbf{G}'_{zy}$	0.00	$\mathbf{A}_{zy}$	0.00	$\mathbf{A}_{y,zz}$	0.00
$\mathbf{g}_{zz}$	0.06	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	0.11	$\mathbf{A}_{z,zz}$	0.00
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	0.00
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	0.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.00
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	0.00
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	-0.11
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.00
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	0.00
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-250.96
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	0.00

S111. Dominant Excited State Data for 12 Using 6-311+G:**

State Number: 1

Excited State Wavelength: 459.83nm

Velocity Oscillator Strength: 0.2817

Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	0.0018	$(\mathbf{r} \times \nabla)_x$	1.5575	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	0.0010	$\mathbf{R}_{xx}$	-2.77
∇_y	-0.2046	$(\mathbf{r} \times \nabla)_y$	-0.0037	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	-0.0027	$\mathbf{R}_{xy}$	-0.01
∇_z	-0.0037	$(\mathbf{r} \times \nabla)_z$	0.0034	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	-0.0075	$\mathbf{R}_{xz}$	-0.73
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	-0.0027	$\mathbf{R}_{yx}$	1452.44
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	0.0384	$\mathbf{R}_{yy}$	12.93
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	0.4330	$\mathbf{R}_{yz}$	4.23
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	-0.0075	$\mathbf{R}_{zx}$	24.61
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	0.4330	$\mathbf{R}_{zy}$	-0.06
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	0.0134	$\mathbf{R}_{zz}$	15.47
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.85	$\mathbf{G}'_{xx}$	-0.44	$\mathbf{A}_{xx}$	9.95	$\mathbf{A}_{x,xx}$	0.01
$\mathbf{g}_{xy}$	-221.50	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-577.48	$\mathbf{A}_{y,xx}$	-1.34
$\mathbf{g}_{xz}$	-3.64	$\mathbf{G}'_{xz}$	-0.00	$\mathbf{A}_{xz}$	-7.44	$\mathbf{A}_{z,xx}$	-0.02
$\mathbf{g}_{yx}$	-221.50	$\mathbf{G}'_{yx}$	49.92	$\mathbf{A}_{yx}$	0.06	$\mathbf{A}_{x,yy}$	0.45
$\mathbf{g}_{yy}$	-3.87	$\mathbf{G}'_{yy}$	-0.12	$\mathbf{A}_{yy}$	-5.02	$\mathbf{A}_{y,yy}$	-51.30
$\mathbf{g}_{yz}$	-0.63	$\mathbf{G}'_{yz}$	0.11	$\mathbf{A}_{yz}$	0.02	$\mathbf{A}_{z,yy}$	-0.93
$\mathbf{g}_{zx}$	-3.64	$\mathbf{G}'_{zx}$	0.90	$\mathbf{A}_{zx}$	1.30	$\mathbf{A}_{x,zz}$	0.16
$\mathbf{g}_{zy}$	-0.63	$\mathbf{G}'_{zy}$	-0.00	$\mathbf{A}_{zy}$	-3.16	$\mathbf{A}_{y,zz}$	-17.90
$\mathbf{g}_{zz}$	-1.63	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	-4.93	$\mathbf{A}_{z,zz}$	-0.32
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	-0.03
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	3.61
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.07
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-0.09
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	10.02
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.18
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	5.09
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-578.41
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	-10.46

S112. Dominant Excited State Data for 12 Using aug-cc-pVDZ:

State Number: 1

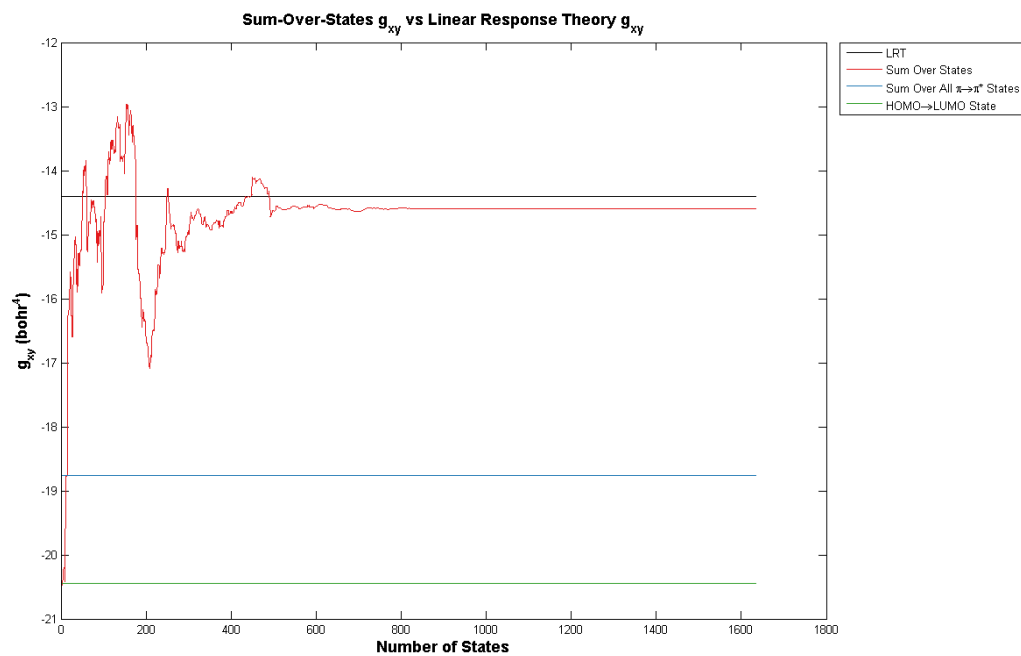
Excited State Wavelength: 464.03nm

Velocity Oscillator Strength: 0.2458

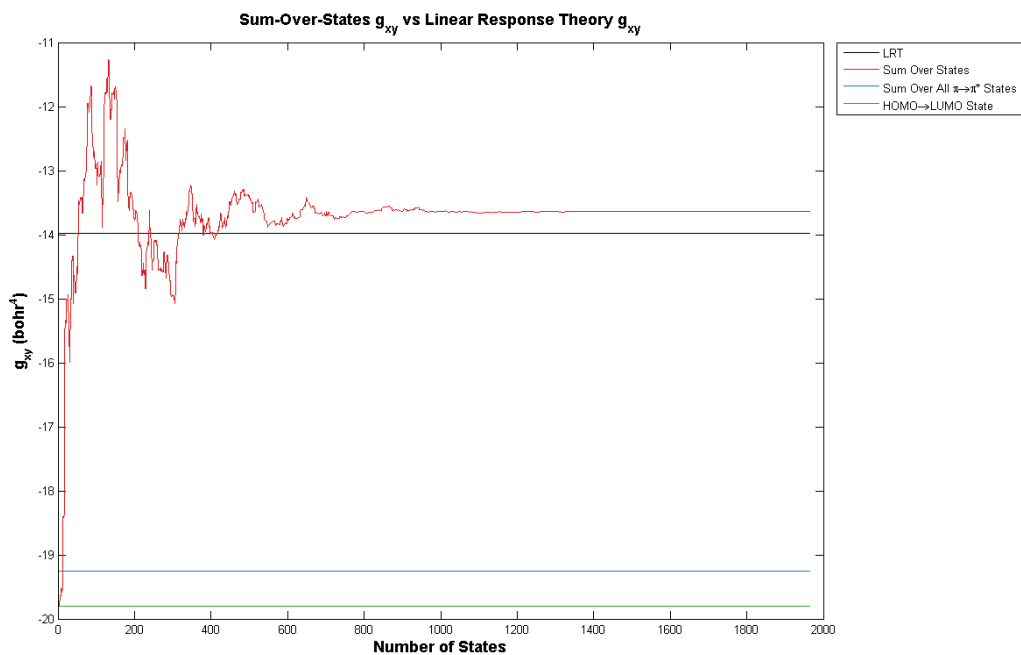
Dominant Transition:

∇_α		$(\mathbf{r} \times \nabla)_\alpha$		$(\mathbf{r} \nabla + \nabla \mathbf{r})_{\alpha\beta}$		$\mathbf{R}_{\alpha\beta}$	
∇_x	-0.0018	$(\mathbf{r} \times \nabla)_x$	-1.5461	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xx}$	-0.0011	$\mathbf{R}_{xx}$	-2.17
∇_y	0.1902	$(\mathbf{r} \times \nabla)_y$	0.0037	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xy}$	0.0023	$\mathbf{R}_{xy}$	-0.01
∇_z	0.0038	$(\mathbf{r} \times \nabla)_z$	-0.0037	$(\mathbf{r} \nabla + \nabla \mathbf{r})_{xz}$	0.0069	$\mathbf{R}_{xz}$	-0.74
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yx}$	0.0023	$\mathbf{R}_{yx}$	1350.00
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yy}$	-0.0346	$\mathbf{R}_{yy}$	12.37
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{yz}$	-0.4253	$\mathbf{R}_{yz}$	3.94
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zx}$	0.0069	$\mathbf{R}_{zx}$	24.12
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zy}$	-0.4253	$\mathbf{R}_{zy}$	-0.06
				$(\mathbf{r} \nabla + \nabla \mathbf{r})_{zz}$	-0.0131	$\mathbf{R}_{zz}$	14.35
$\mathbf{g}_{\alpha\beta}$		$\mathbf{G}'_{\alpha\beta}$		$\mathbf{A}_{\alpha\beta}$		$\mathbf{A}_{\alpha,\beta\gamma}$	
$\mathbf{g}_{xx}$	0.70	$\mathbf{G}'_{xx}$	-0.46	$\mathbf{A}_{xx}$	8.93	$\mathbf{A}_{x,xx}$	0.01
$\mathbf{g}_{xy}$	-213.96	$\mathbf{G}'_{xy}$	0.00	$\mathbf{A}_{xy}$	-553.20	$\mathbf{A}_{y,xx}$	-1.43
$\mathbf{g}_{xz}$	-3.73	$\mathbf{G}'_{xz}$	-0.00	$\mathbf{A}_{xz}$	-6.00	$\mathbf{A}_{z,xx}$	-0.03
$\mathbf{g}_{yx}$	-213.96	$\mathbf{G}'_{yx}$	48.33	$\mathbf{A}_{yx}$	0.06	$\mathbf{A}_{x,yy}$	0.43
$\mathbf{g}_{yy}$	-4.03	$\mathbf{G}'_{yy}$	-0.12	$\mathbf{A}_{yy}$	-5.18	$\mathbf{A}_{y,yy}$	-45.08
$\mathbf{g}_{yz}$	-0.61	$\mathbf{G}'_{yz}$	0.12	$\mathbf{A}_{yz}$	0.02	$\mathbf{A}_{z,yy}$	-0.90
$\mathbf{g}_{zx}$	-3.73	$\mathbf{G}'_{zx}$	0.97	$\mathbf{A}_{zx}$	1.40	$\mathbf{A}_{x,zz}$	0.16
$\mathbf{g}_{zy}$	-0.61	$\mathbf{G}'_{zy}$	-0.00	$\mathbf{A}_{zy}$	-2.57	$\mathbf{A}_{y,zz}$	-17.07
$\mathbf{g}_{zz}$	-1.41	$\mathbf{G}'_{zz}$	0.00	$\mathbf{A}_{zz}$	-3.75	$\mathbf{A}_{z,zz}$	-0.34
						$\mathbf{A}_{x,xy}, \mathbf{A}_{x,yx}$	-0.03
						$\mathbf{A}_{y,xy}, \mathbf{A}_{y,yx}$	3.00
						$\mathbf{A}_{z,xy}, \mathbf{A}_{z,yx}$	0.06
						$\mathbf{A}_{x,xz}, \mathbf{A}_{x,zx}$	-0.09
						$\mathbf{A}_{y,xz}, \mathbf{A}_{y,zx}$	8.99
						$\mathbf{A}_{z,xz}, \mathbf{A}_{z,zx}$	0.18
						$\mathbf{A}_{x,yz}, \mathbf{A}_{x,zy}$	5.24
						$\mathbf{A}_{y,yz}, \mathbf{A}_{y,zy}$	-554.10
						$\mathbf{A}_{z,yz}, \mathbf{A}_{z,zy}$	-11.07

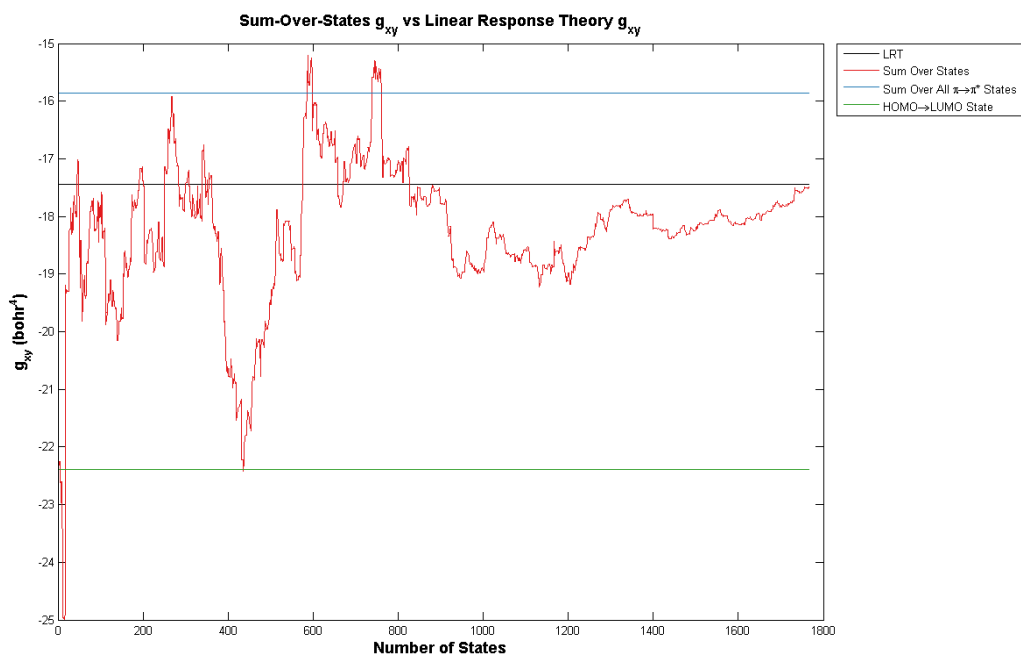
S113. Sum-over-states plot for xy tensor component of I using 6-311+G**



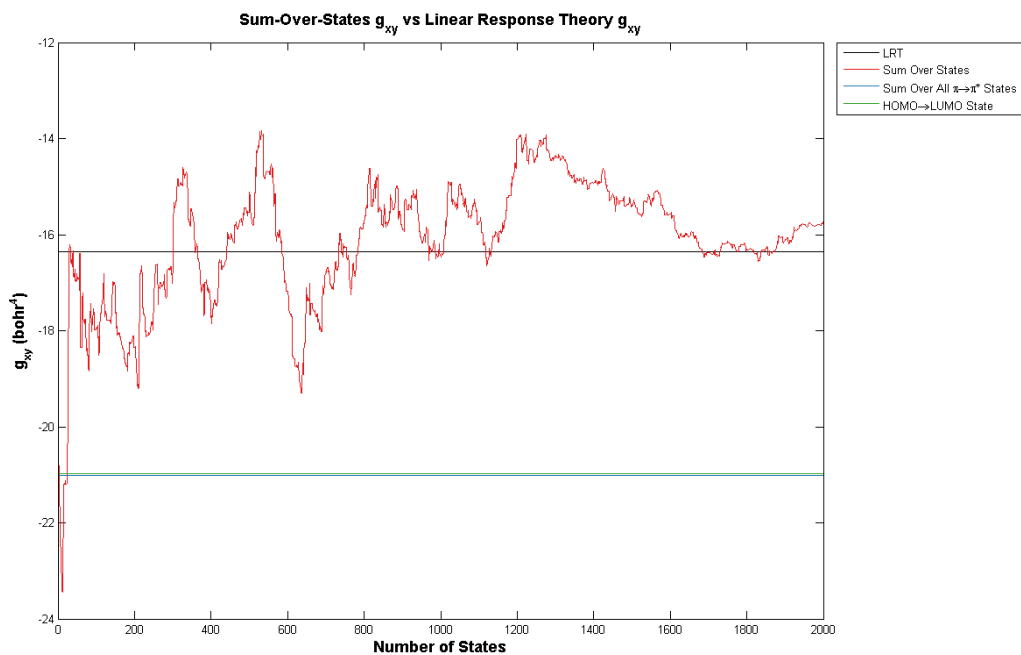
S114. Sum-over-states plot for xy tensor component of I using aug-cc-pVDZ



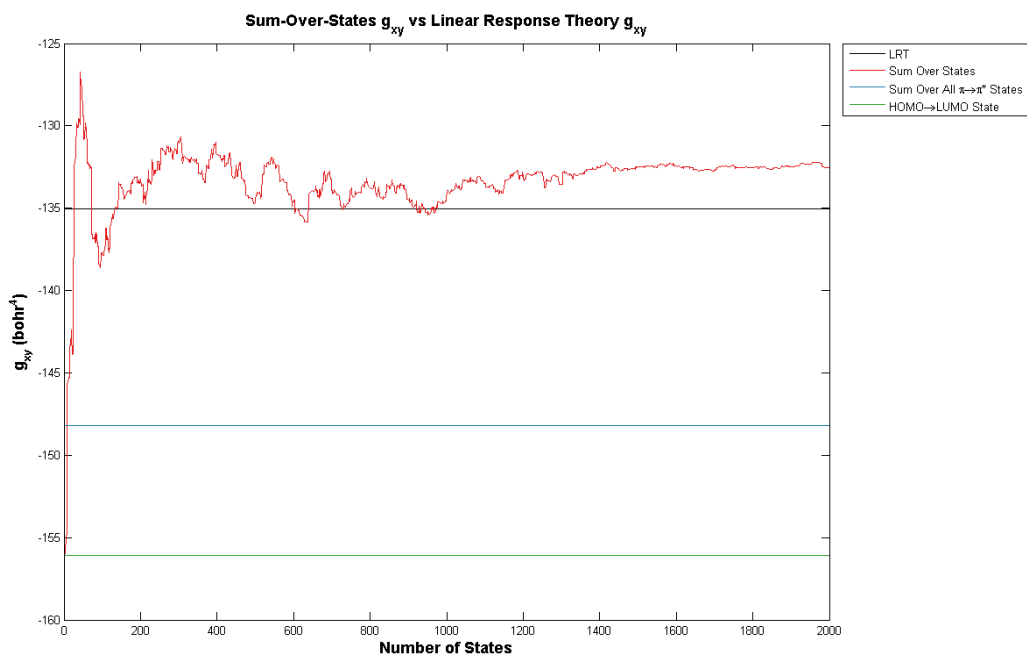
*S115. Sum-over-states plot for xy tensor component of 2 using 6-311+G***



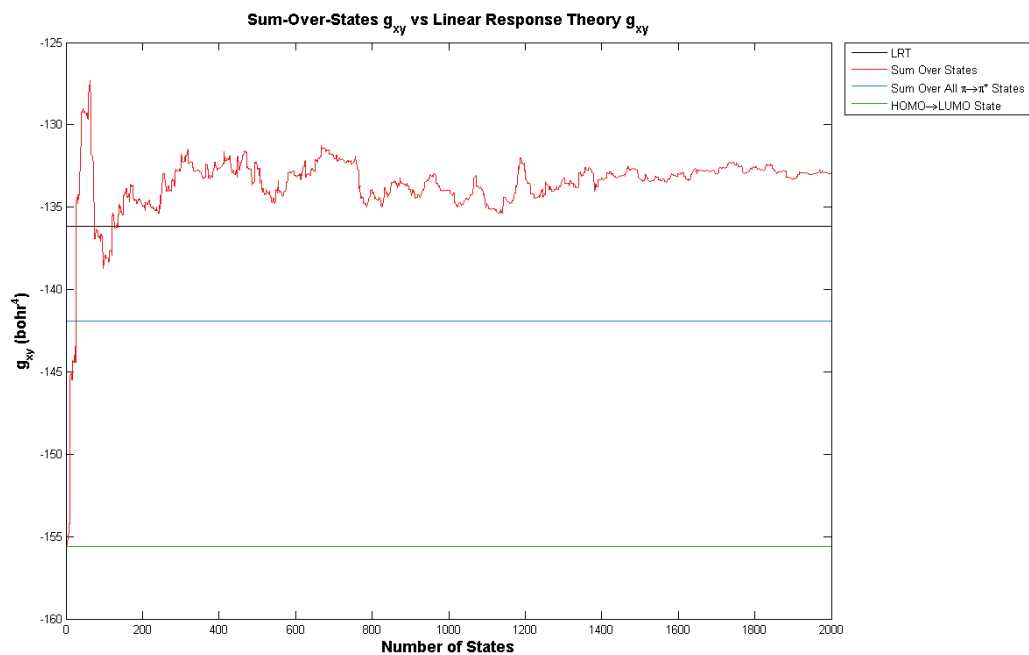
S116. Sum-over-states plot for xy tensor component of 2 using aug-cc-pVDZ



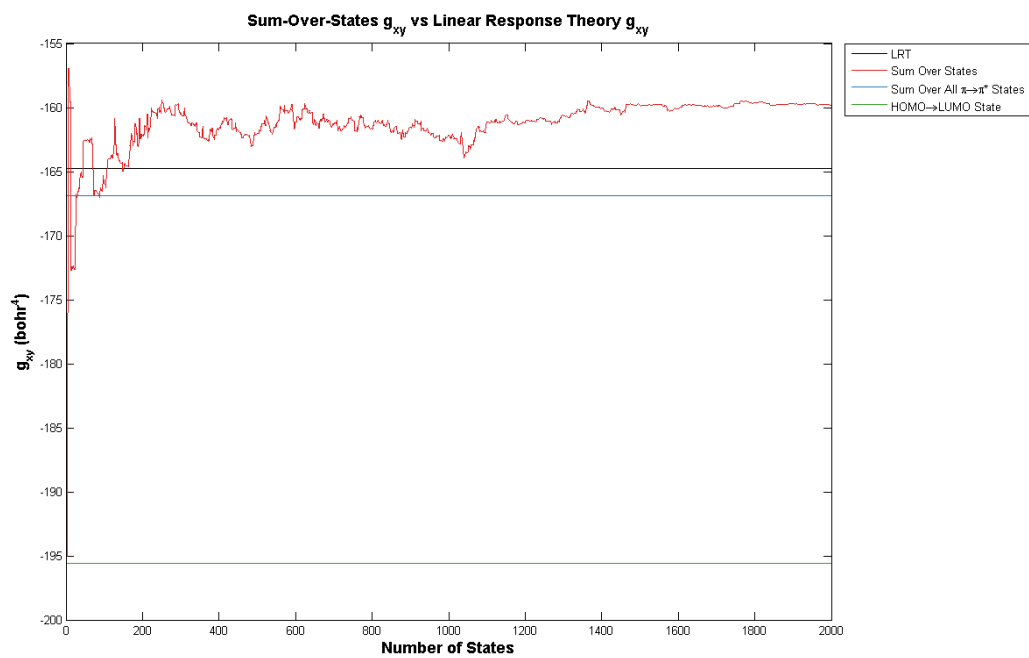
*S117. Sum-over-states plot for xy tensor component of 3 using 6-311+G***



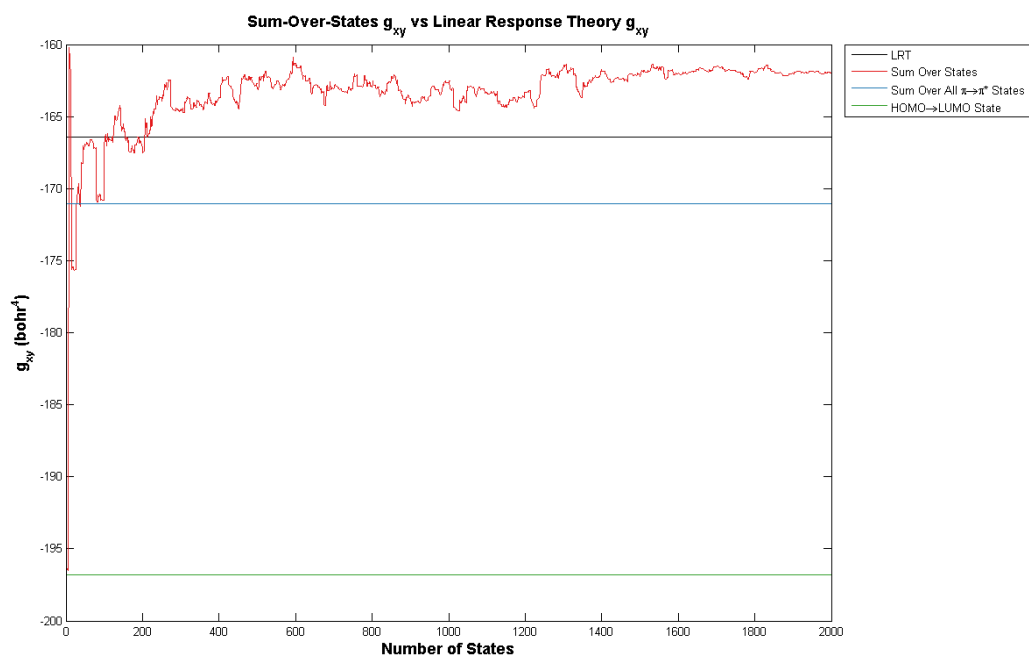
S118. Sum-over-states plot for xy tensor component of 3 using aug-cc-pVDZ



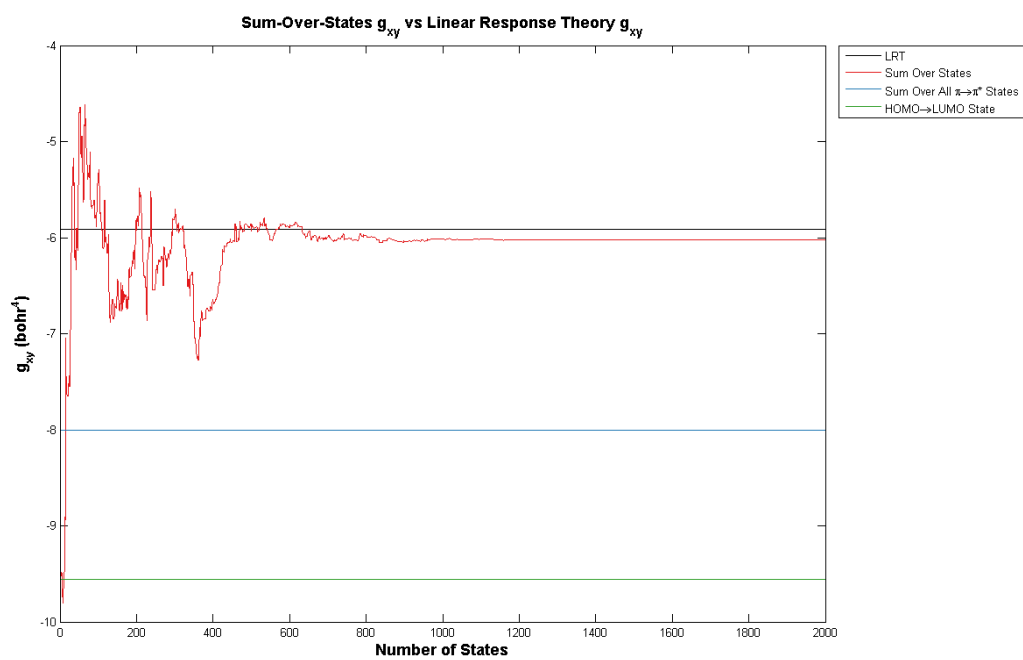
*S119. Sum-over-states plot for xy tensor component of 4 using 6-311+G***



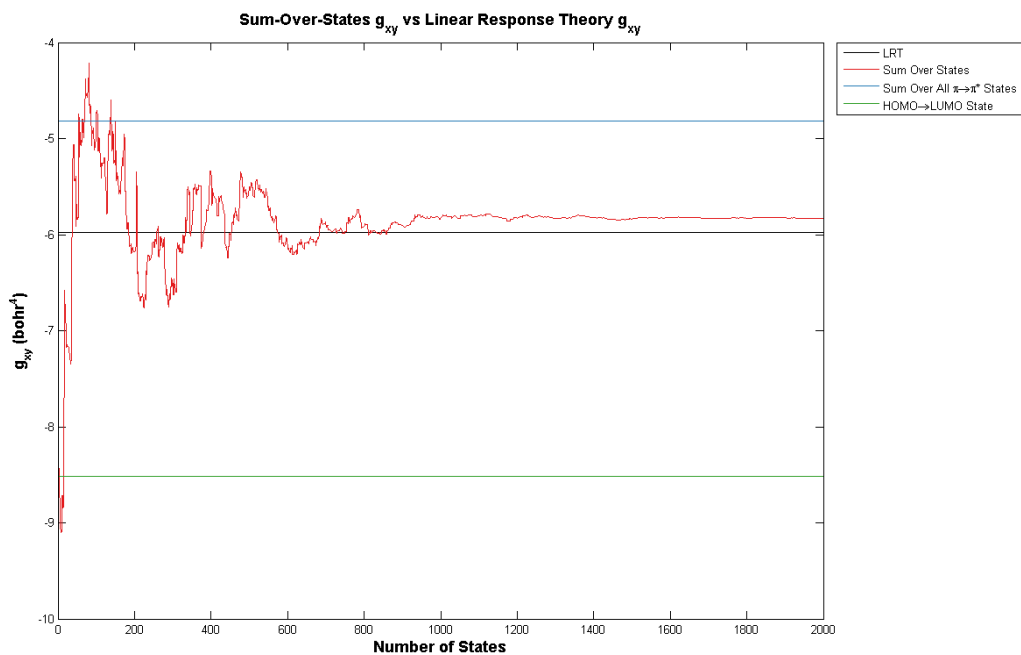
S120. Sum-over-states plot for xy tensor component of 4 using aug-cc-pVDZ



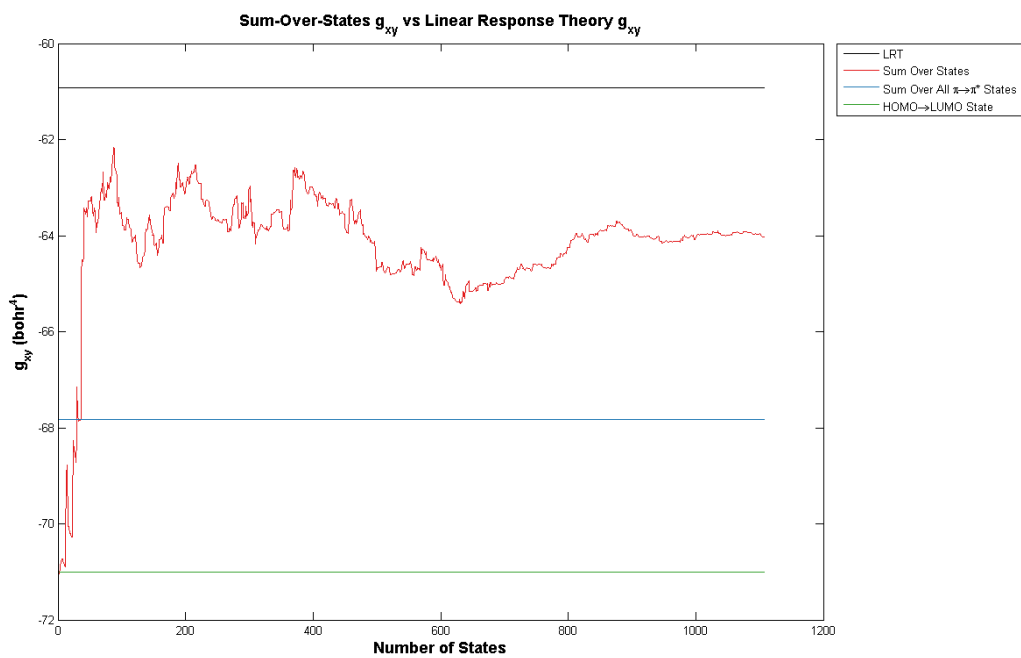
*S121. Sum-over-states plot for xy tensor component of 5 using 6-311+G***



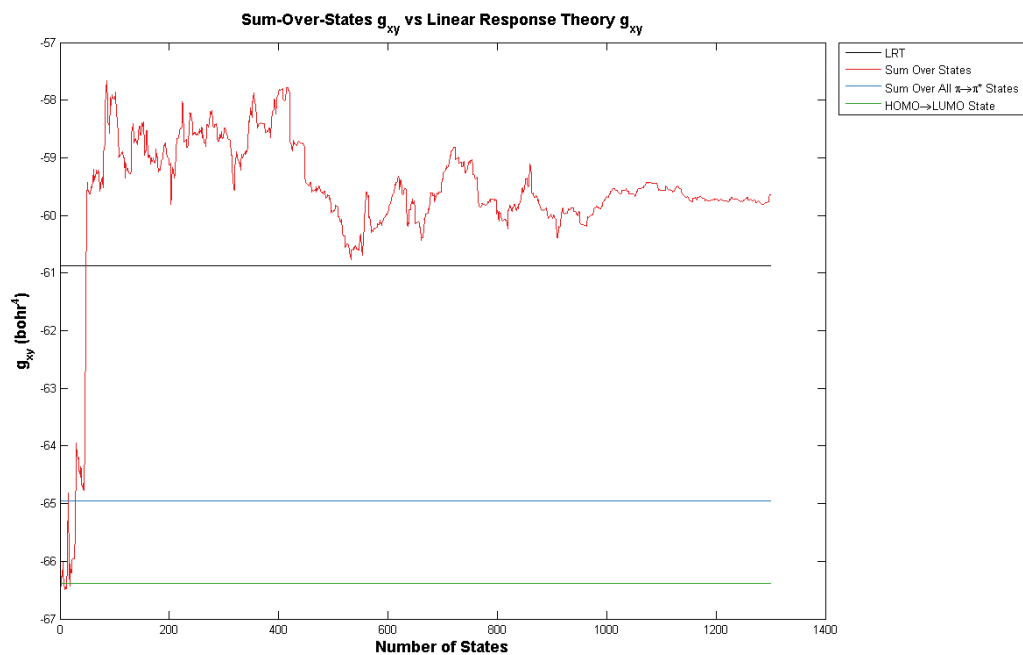
S122. Sum-over-states plot for xy tensor component of 5 using aug-cc-pVDZ



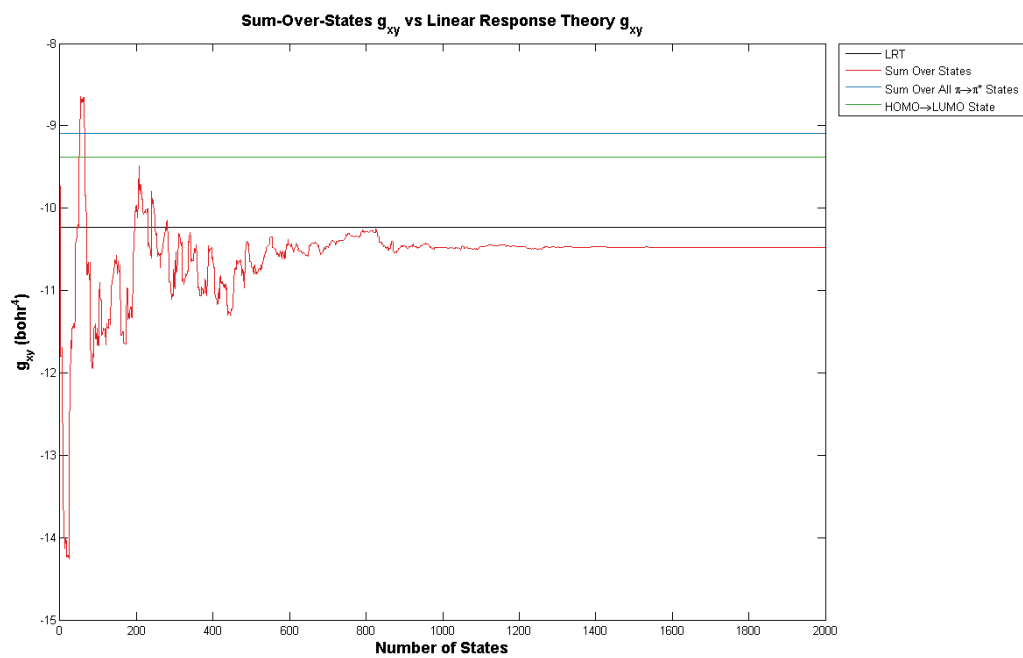
*S123. Sum-over-states plot for xy tensor component of 6 using 6-311+G***



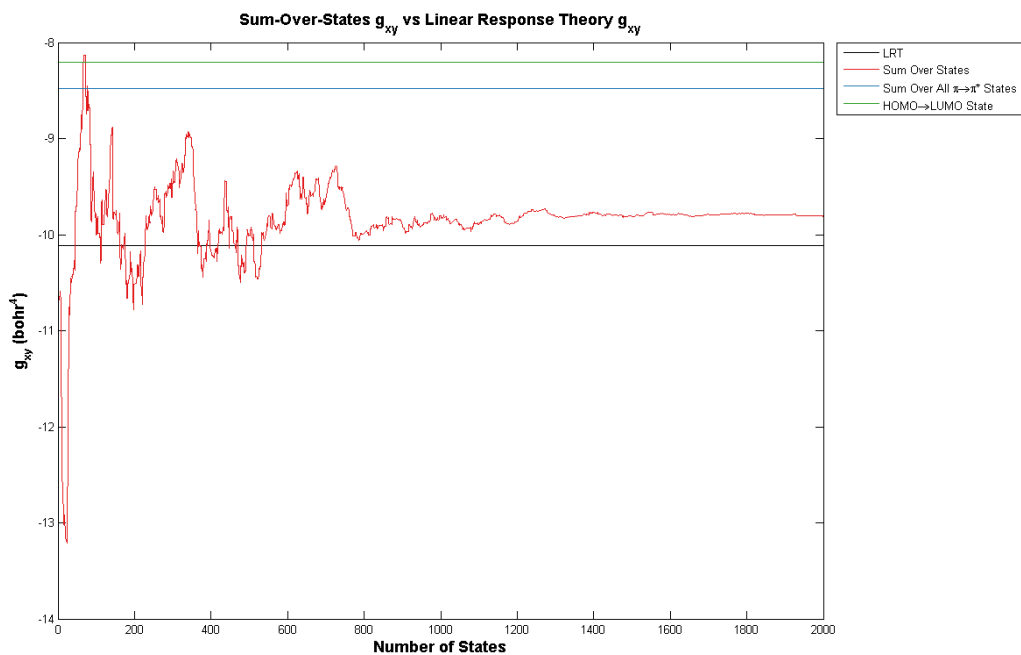
S124. Sum-over-states plot for xy tensor component of 6 using aug-cc-pVDZ



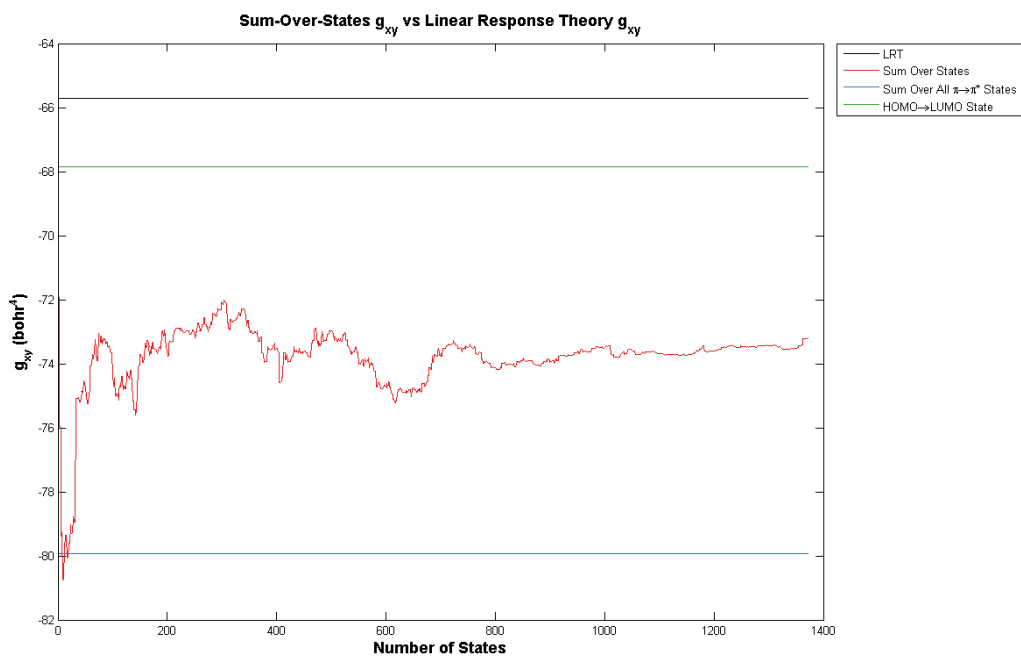
*S125. Sum-over-states plot for xy tensor component of 7 using 6-311+G***



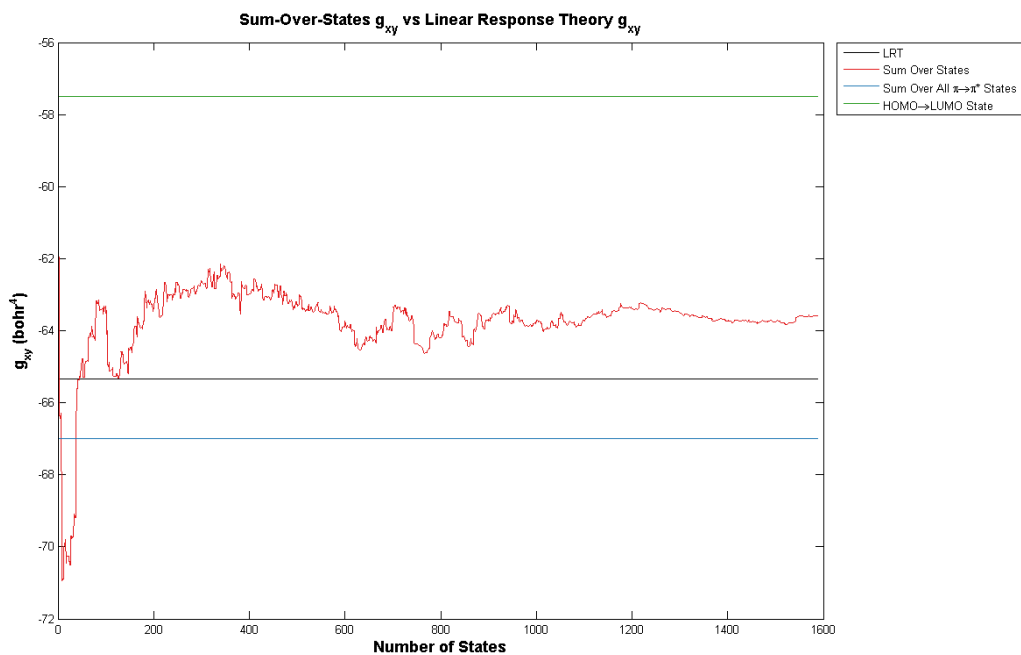
S126. Sum-over-states plot for xy tensor component of 7 using aug-cc-pVDZ



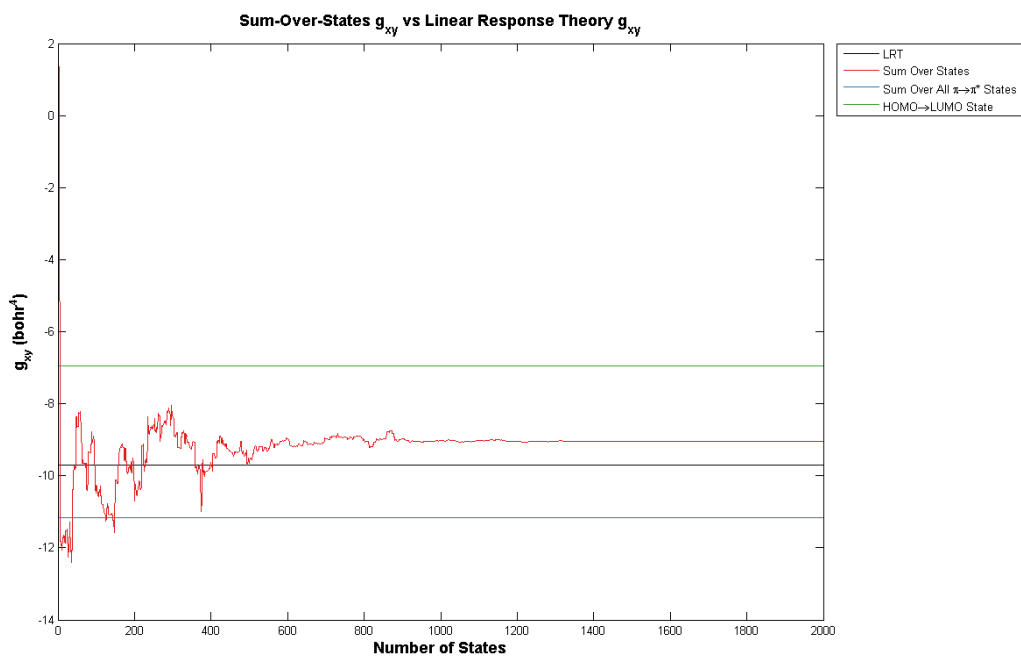
*S127. Sum-over-states plot for xy tensor component of **8** using 6-311+G***



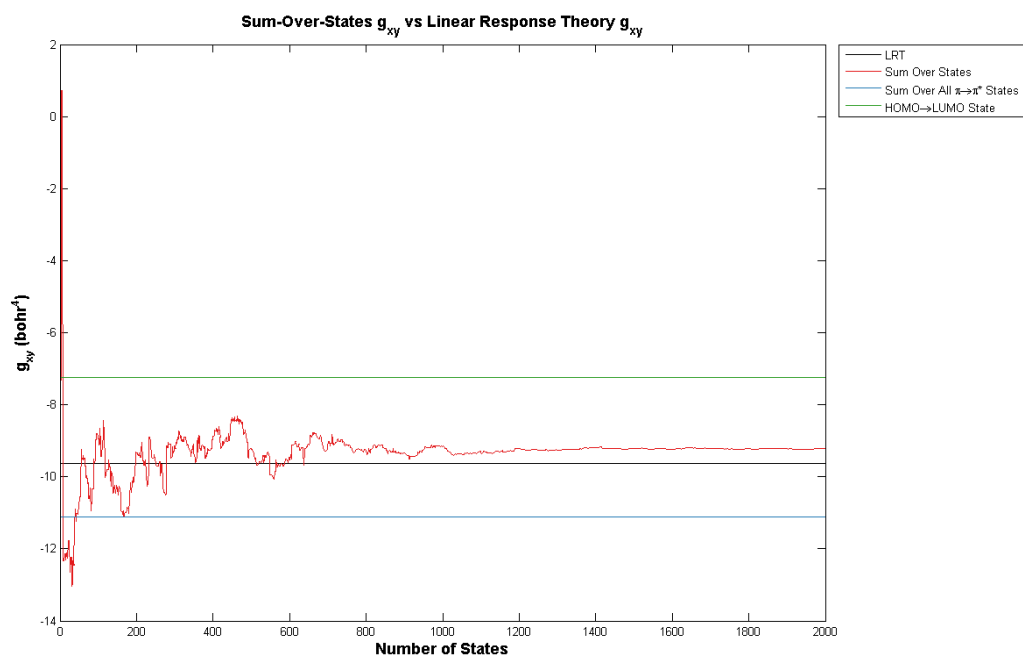
*S128. Sum-over-states plot for xy tensor component of **8** using aug-cc-pVDZ*



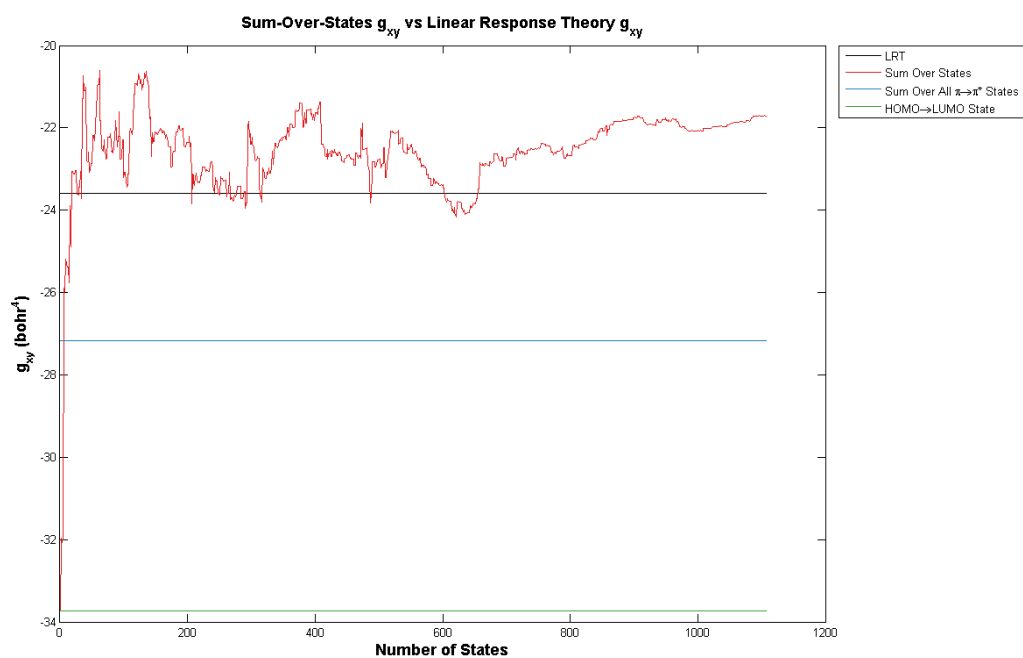
*S129. Sum-over-states plot for xy tensor component of 9 using 6-311+G***



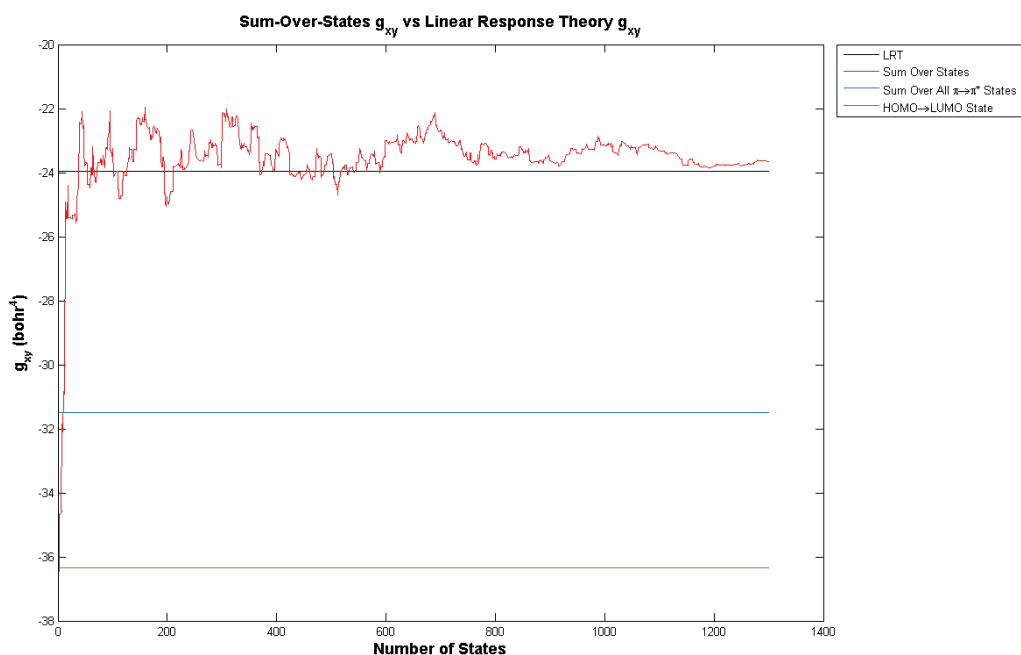
S130. Sum-over-states plot for xy tensor component of 9 using aug-cc-pVDZ



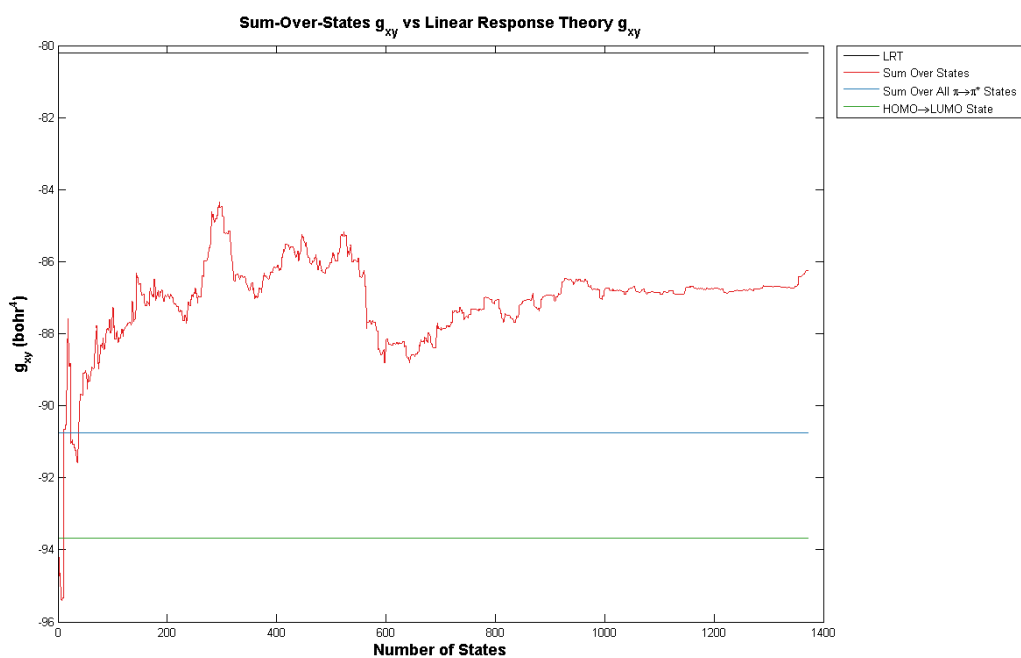
*S131. Sum-over-states plot for xy tensor component of 10 using 6-311+G***



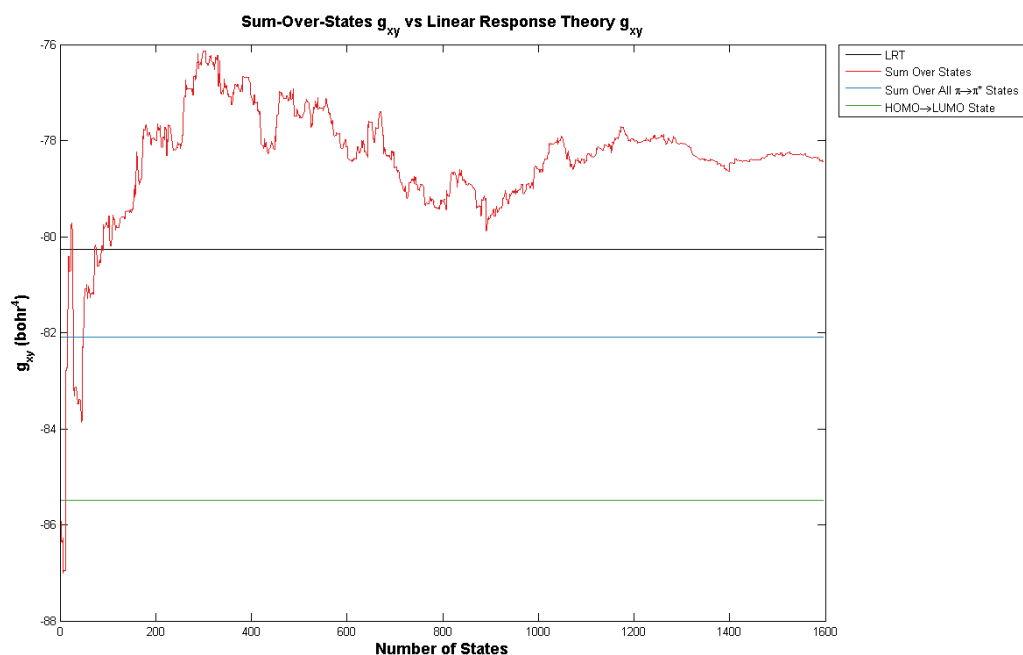
S132. Sum-over-states plot for xy tensor component of 10 using aug-cc-pVDZ



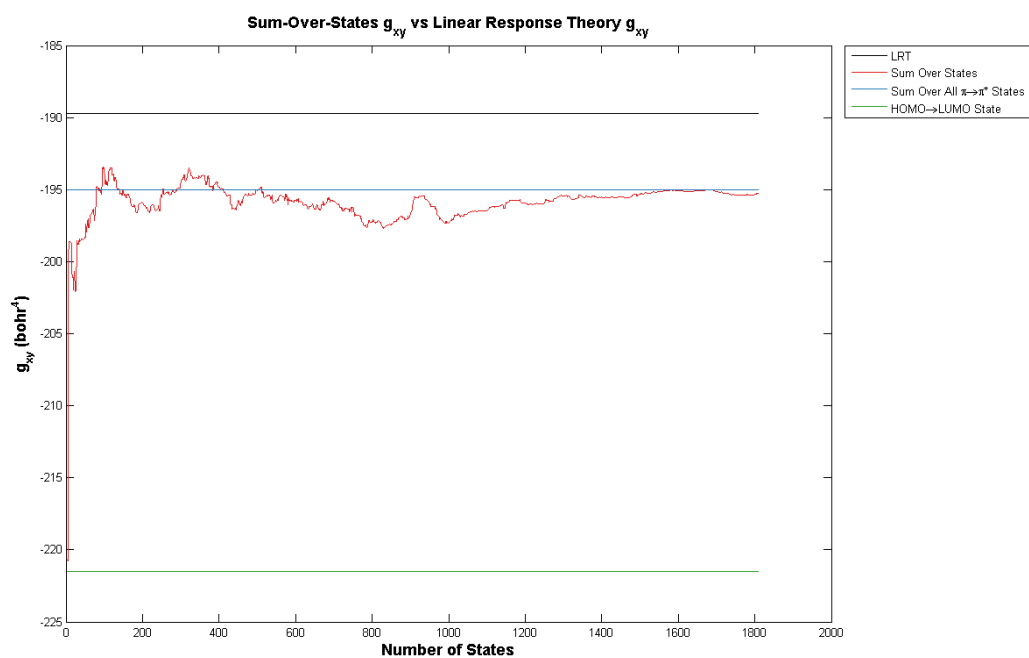
*S133. Sum-over-states plot for xy tensor component of 11 using 6-311+G***



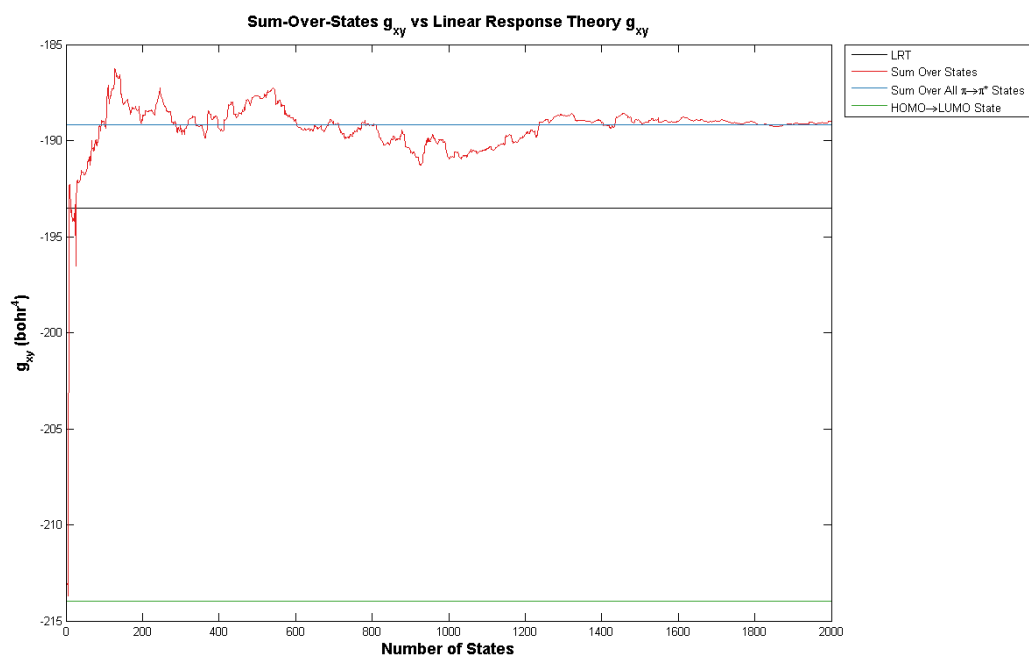
S134. Sum-over-states plot for xy tensor component of 11 using aug-cc-pVDZ



*S135. Sum-over-states plot for xy tensor component of 12 using 6-311+G***

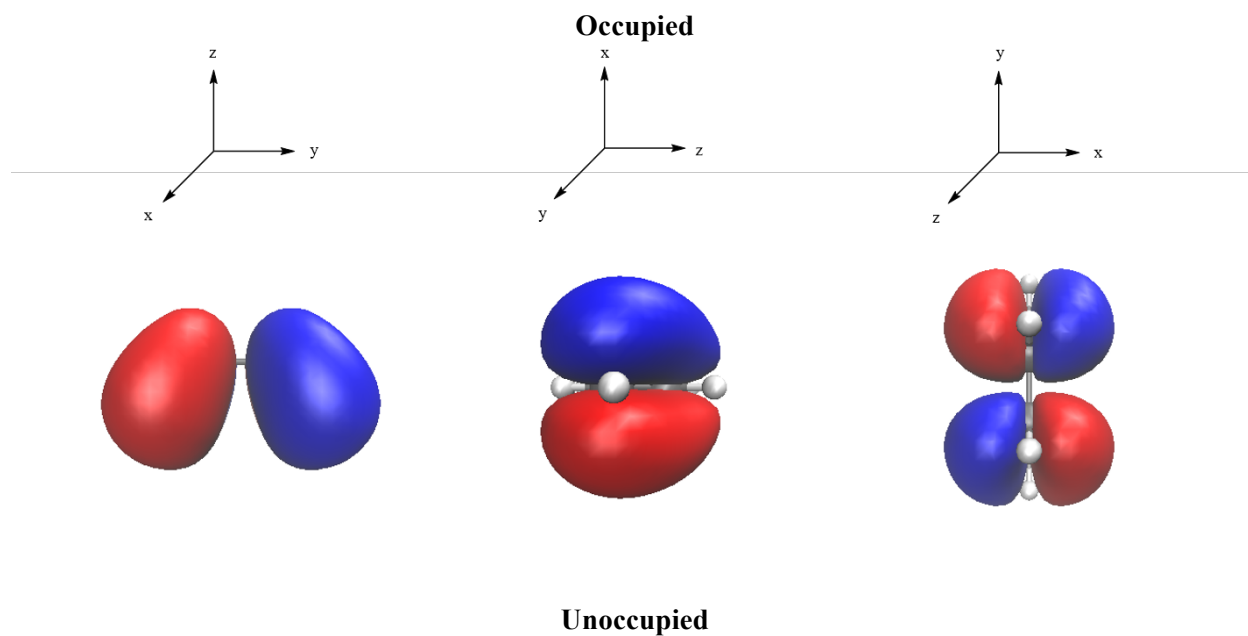


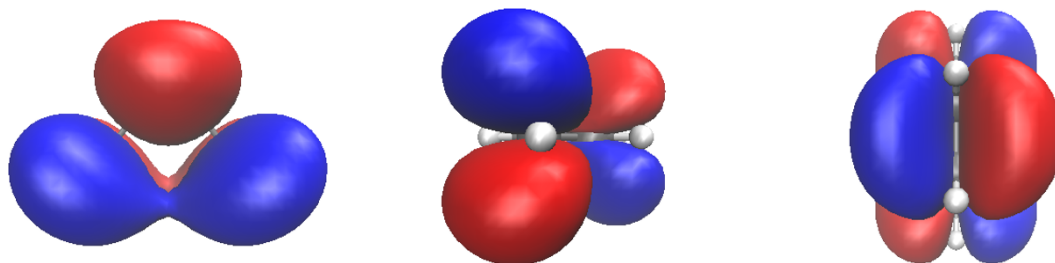
S136. Sum-over-states plot for xy tensor component of 12 using aug-cc-pVDZ



S137. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for **1**

	6-311+G**	aug-cc-pVDZ
Occupied	15	15
Unoccupied	16	16

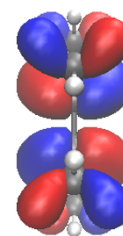
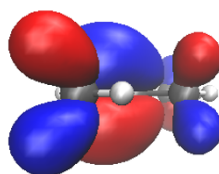
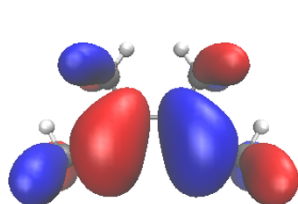
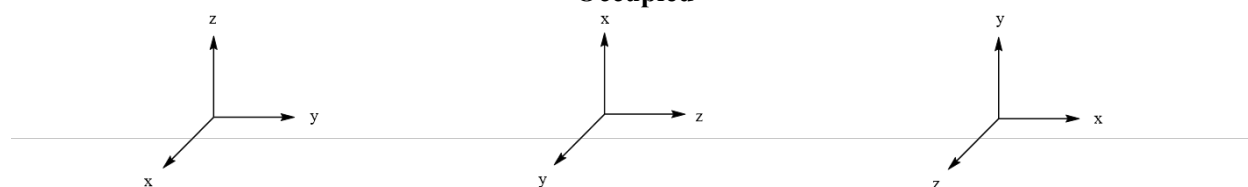




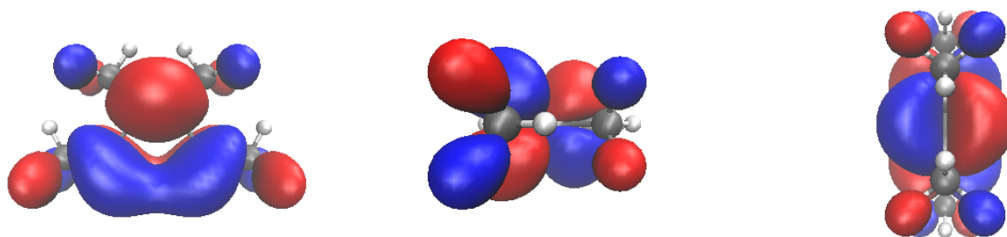
S138. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 2

	6-311+G**	aug-cc-pVDZ
Occupied	31	31
Unoccupied	32	32

Occupied



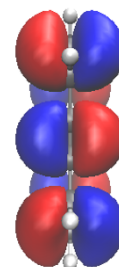
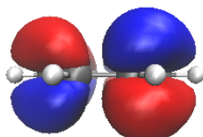
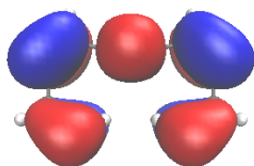
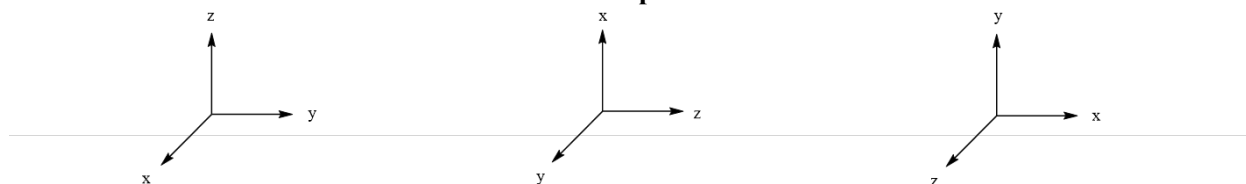
Unoccupied



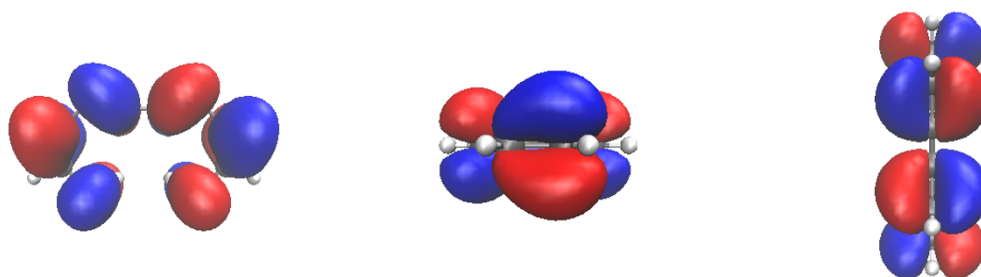
S139. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 3

	6-311+G**	aug-cc-pVDZ
Occupied	35	35
Unoccupied	36	36

Occupied

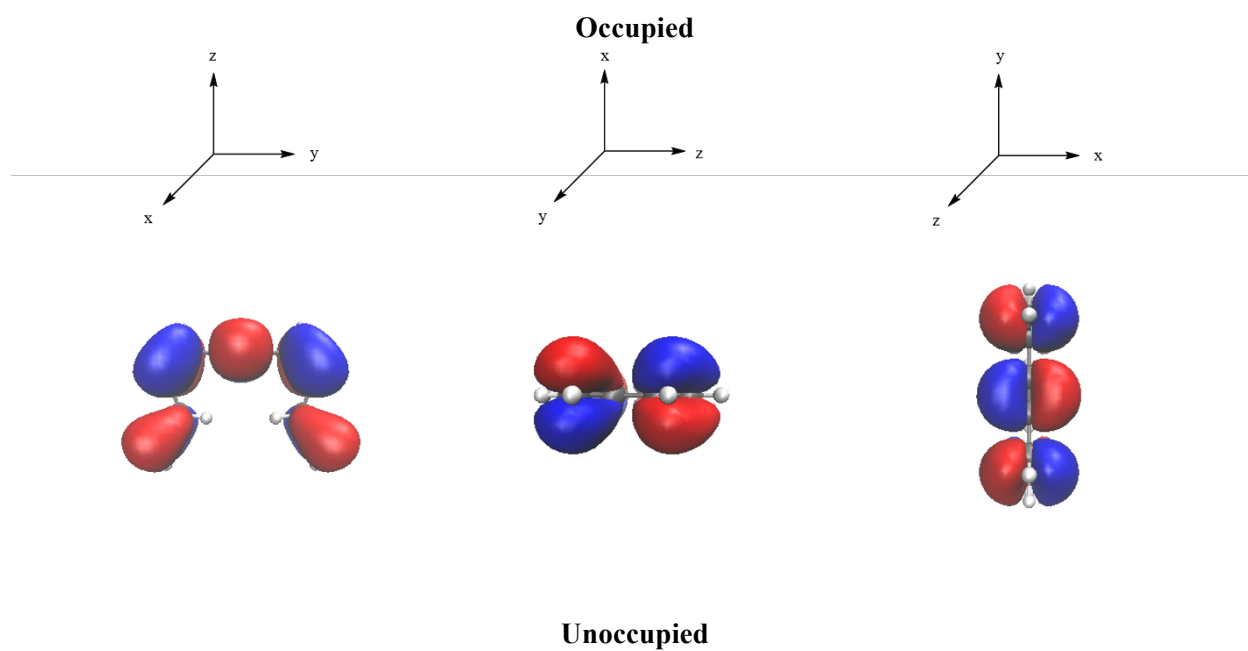


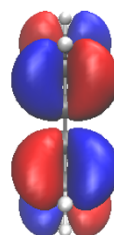
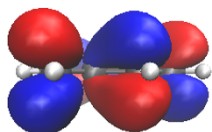
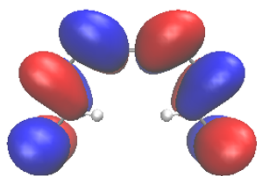
Unoccupied



S140. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 4

	6-311+G**	aug-cc-pVDZ
Occupied	35	35
Unoccupied	36	36

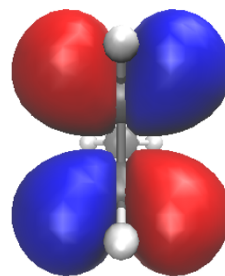
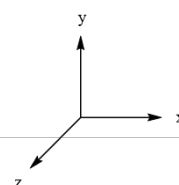
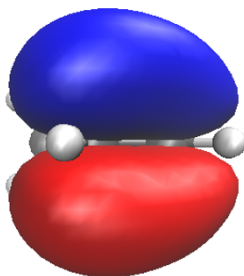
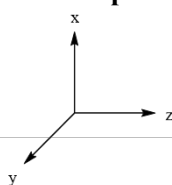
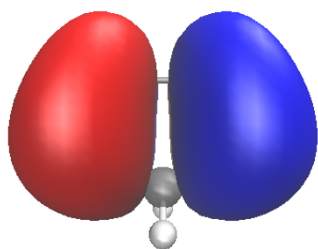
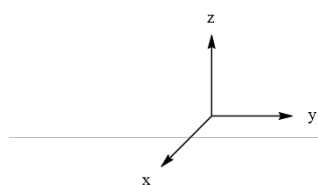




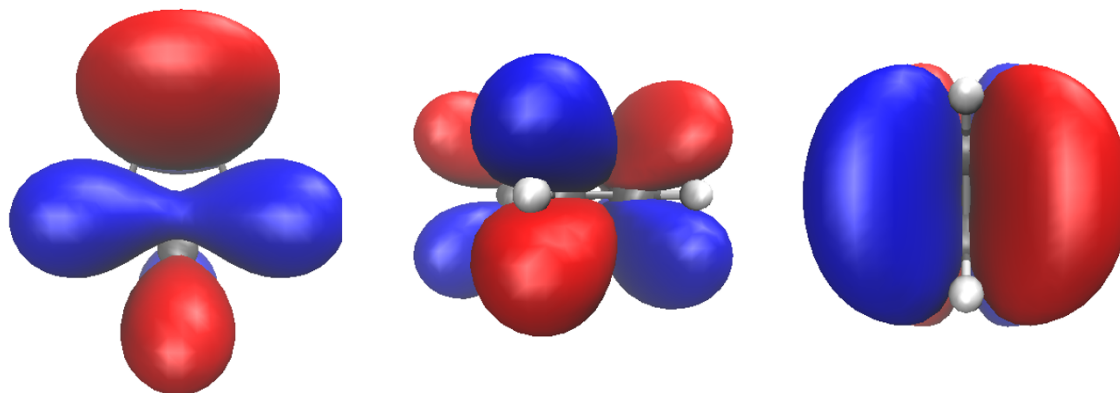
S141. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 5

	6-311+G**	aug-cc-pVDZ
Occupied	18	18
Unoccupied	19	19

Occupied

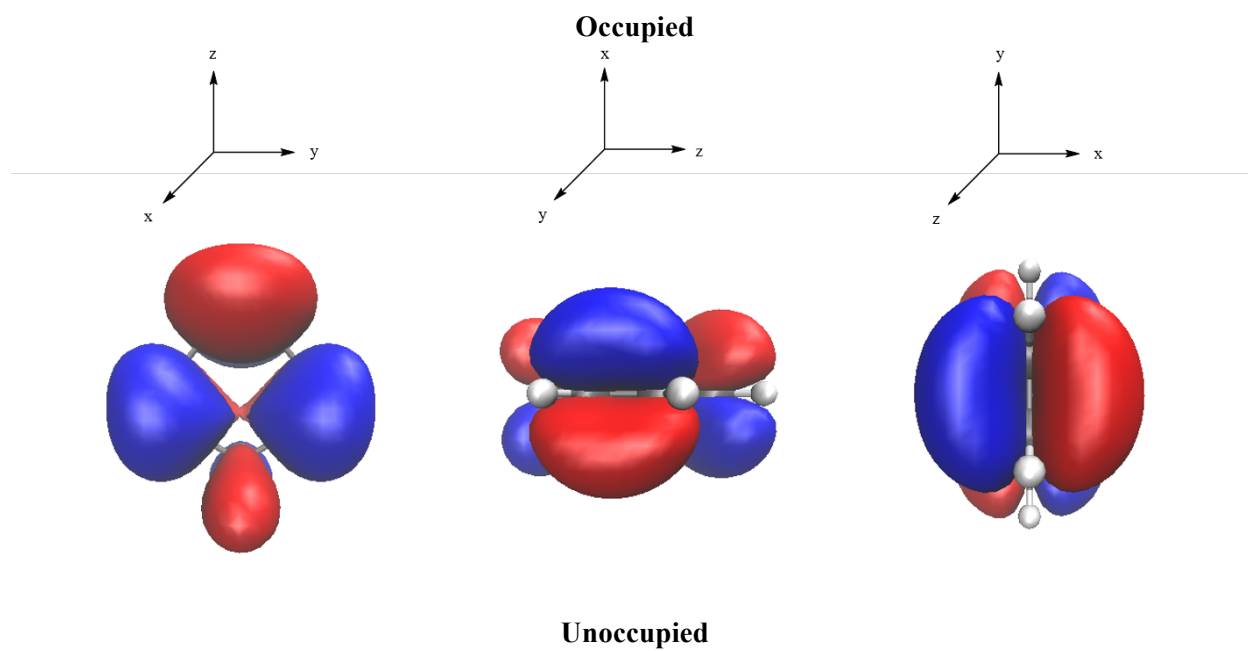


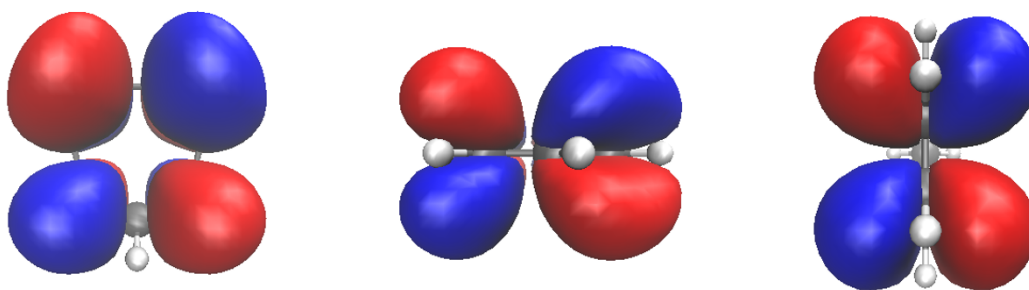
Unoccupied



S142. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 6

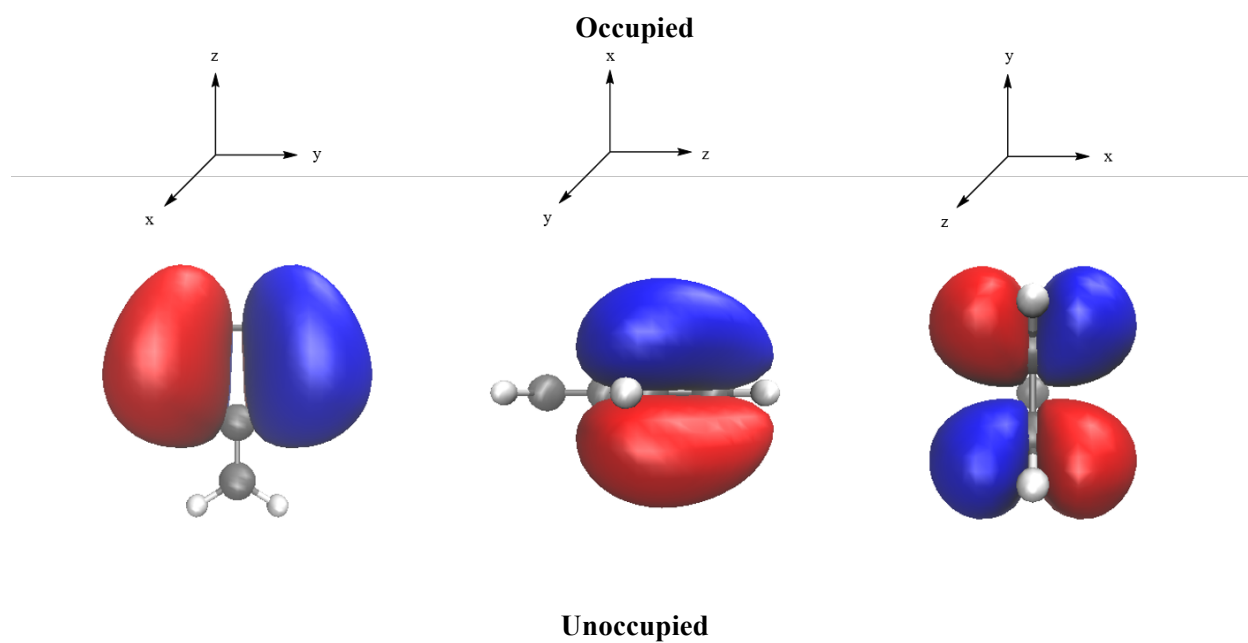
	6-311+G**	aug-cc-pVDZ
Occupied	25	25
Unoccupied	26	26

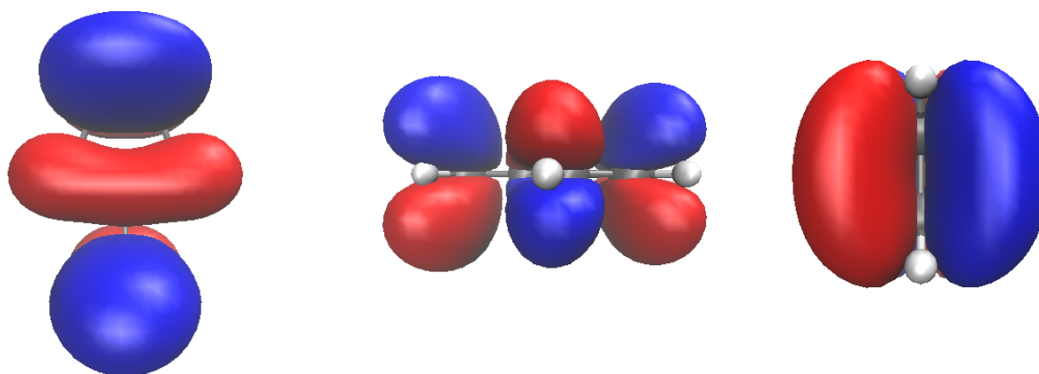




S143. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 7

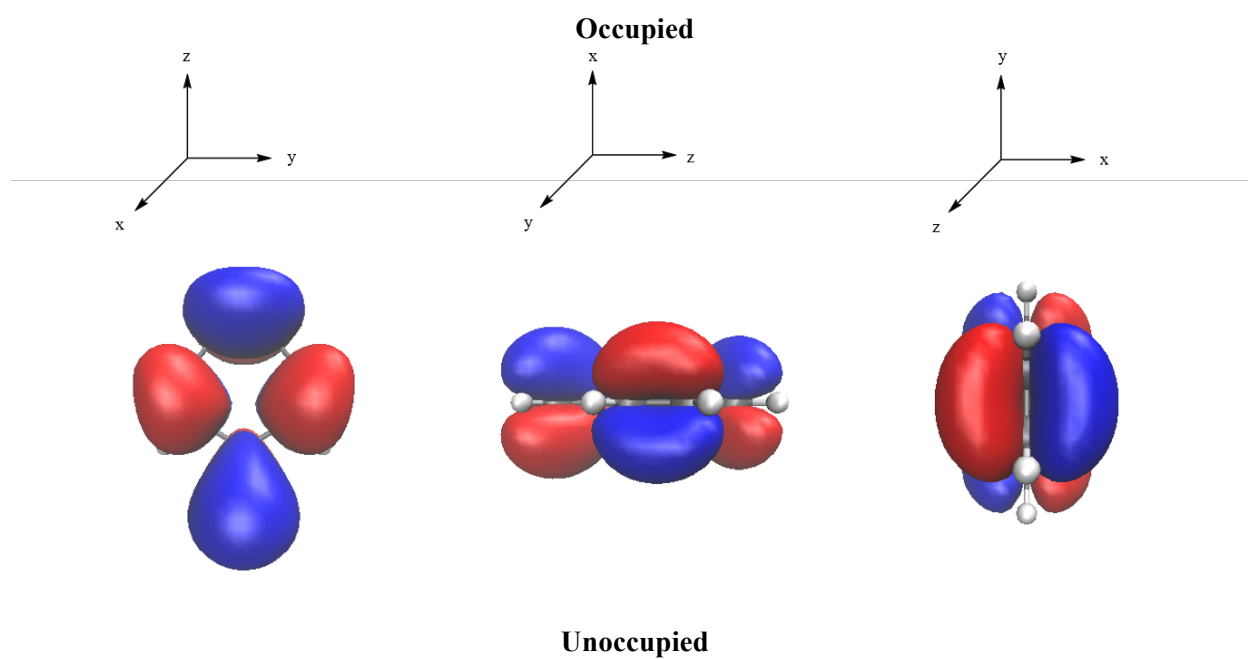
	6-311+G**	aug-cc-pVDZ
Occupied	21	21
Unoccupied	22	22

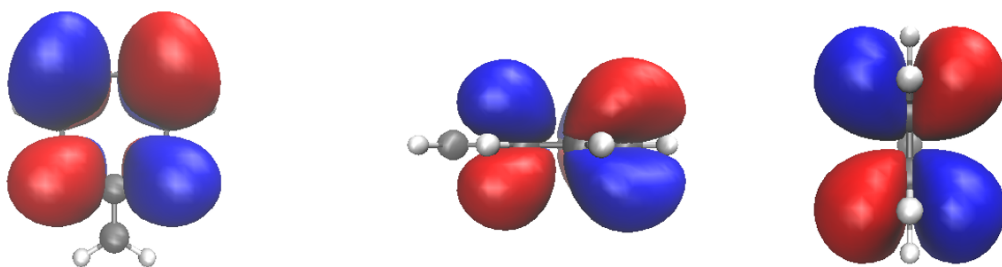




S144. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 8

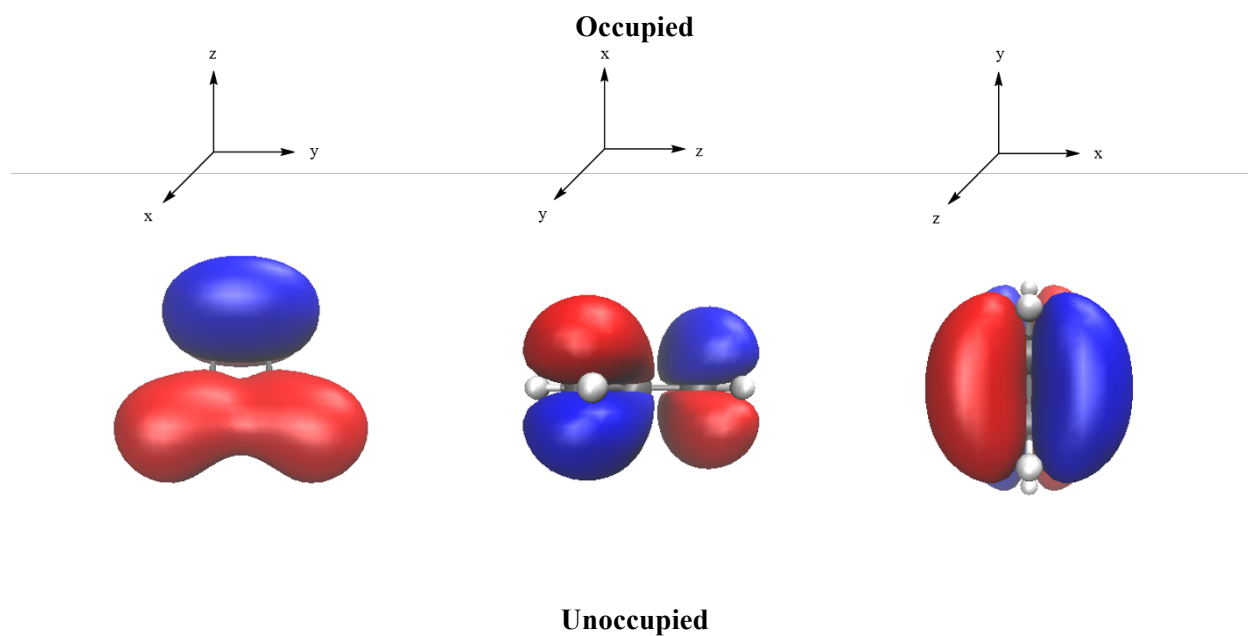
	6-311+G**	aug-cc-pVDZ
Occupied	28	28
Unoccupied	29	29

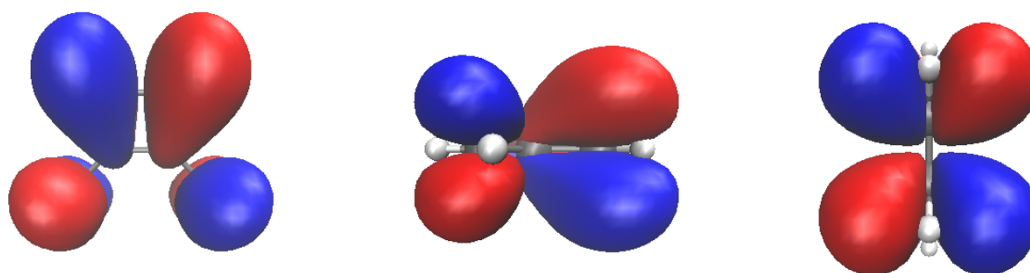




S145. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 9

	6-311+G**	aug-cc-pVDZ
Occupied	21	21
Unoccupied	22	22

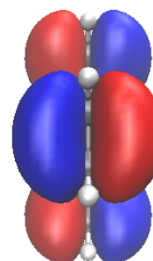
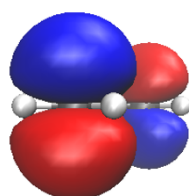
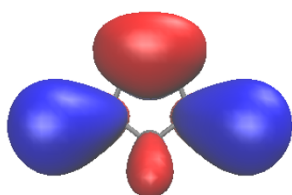
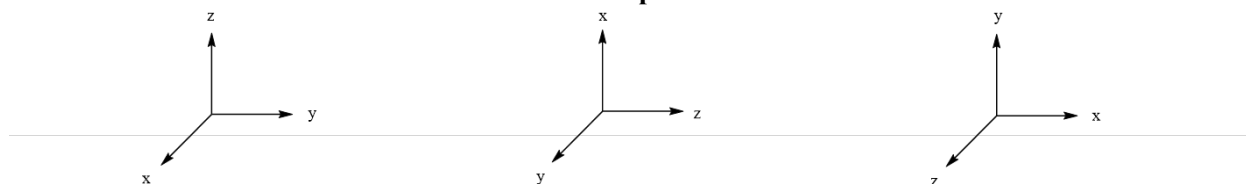




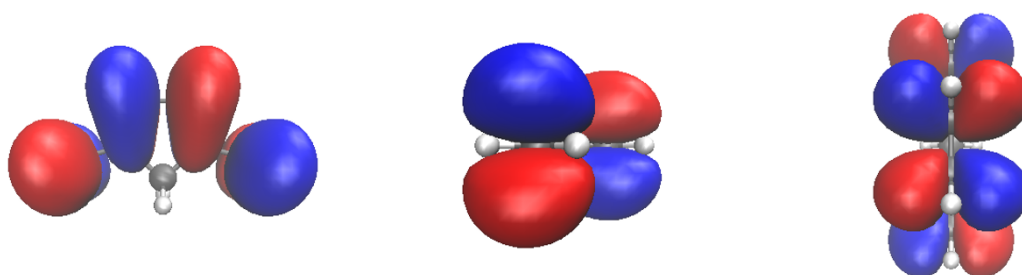
S146. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for **10**

	6-311+G**	aug-cc-pVDZ
Occupied	25	25
Unoccupied	26	26

Occupied

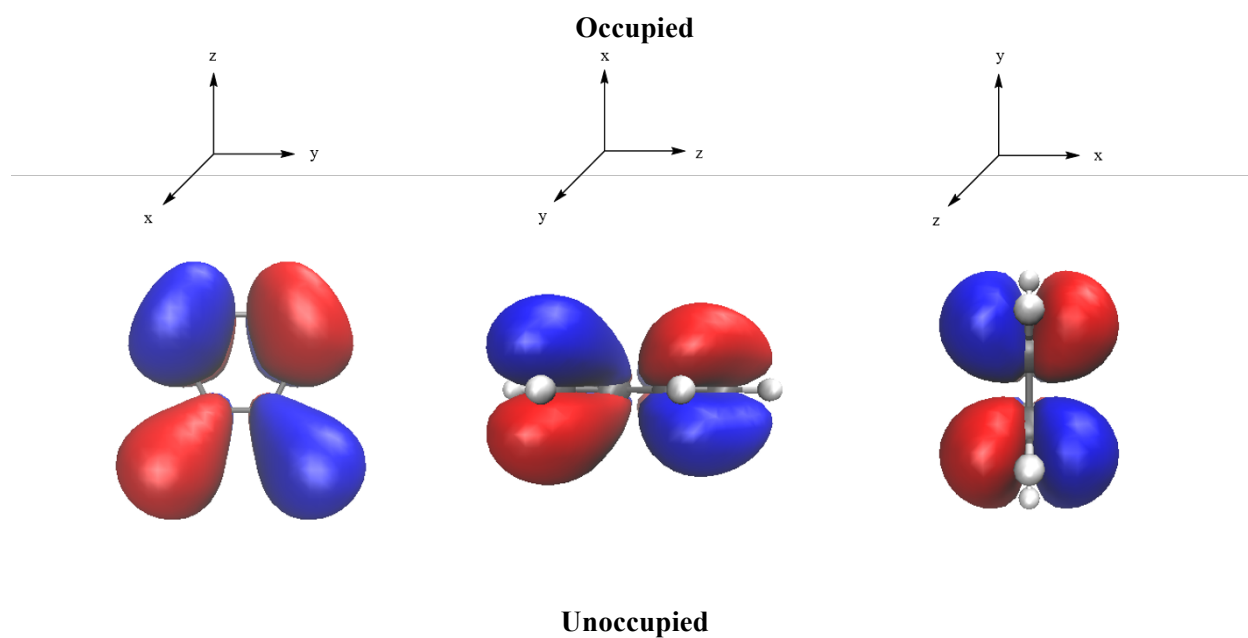


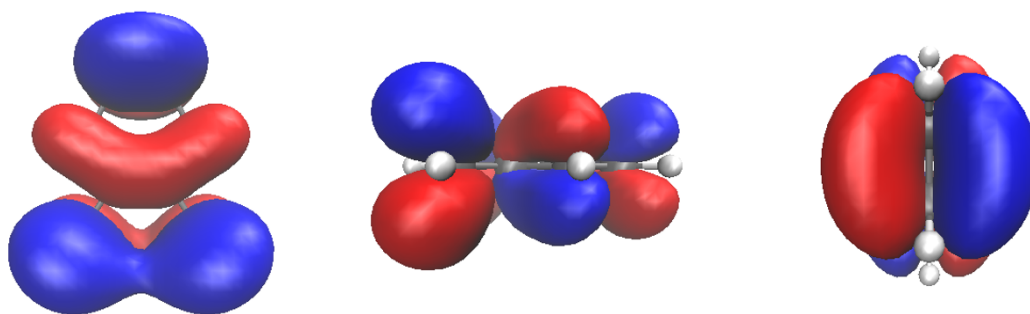
Unoccupied



S147. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 11

	6-311+G**	aug-cc-pVDZ
Occupied	28	28
Unoccupied	29	29

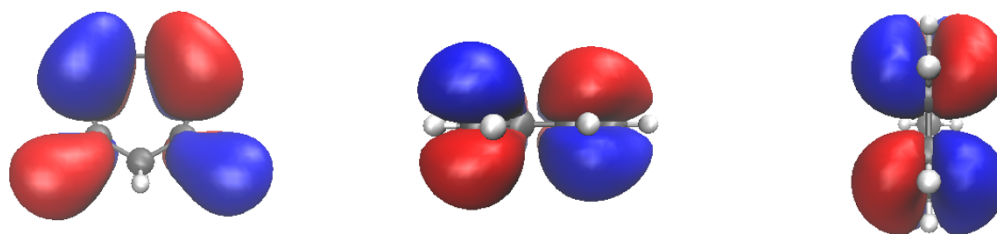
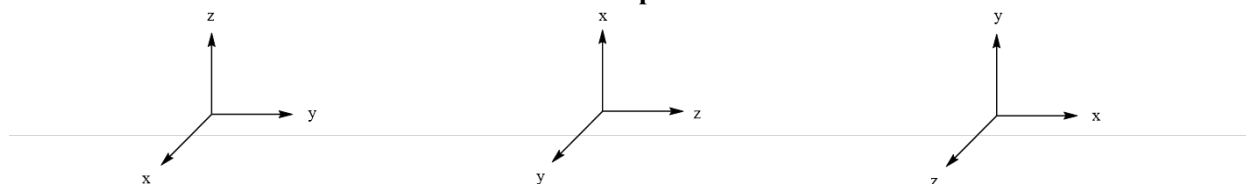




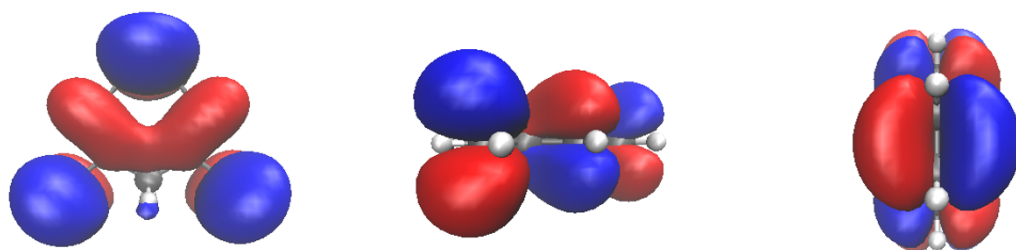
S148. Gaussian generated orbitals corresponding to Hückel HOMO-LUMO transition for 12

	6-311+G**	aug-cc-pVDZ
Occupied	32	32
Unoccupied	33	33

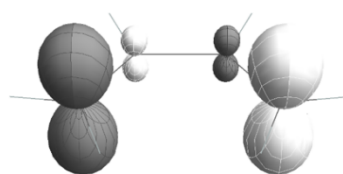
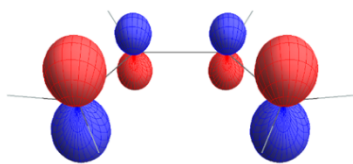
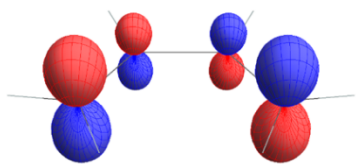
Occupied



Unoccupied



S149. Hückel HOMO and LUMO as well as corresponding overlap density for **1**



$$\pi_2$$

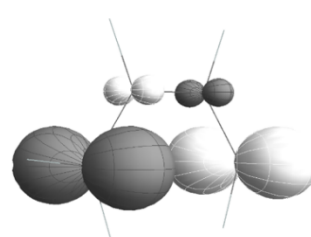
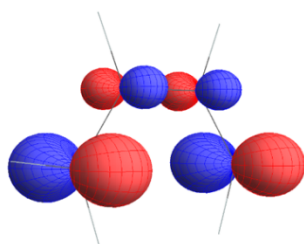
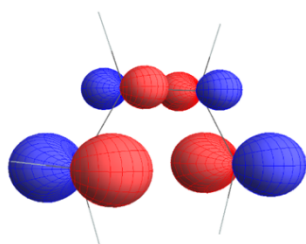
$$\alpha+0.618\beta$$

$$\pi_3^*$$

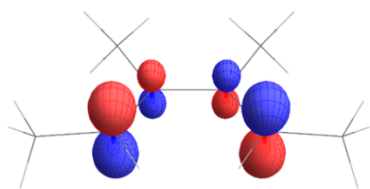
$$\alpha-0.618\beta$$

$$\pi_2 \rightarrow \pi_3^*$$

$$-1.236\beta$$

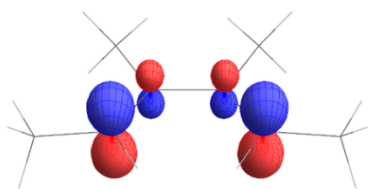


S150. Hückel HOMO and LUMO as well as corresponding overlap density for 2



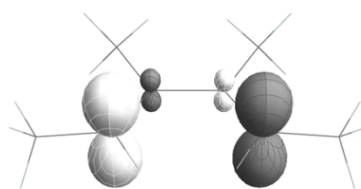
$$\pi_2$$

$$\alpha+0.618\beta$$



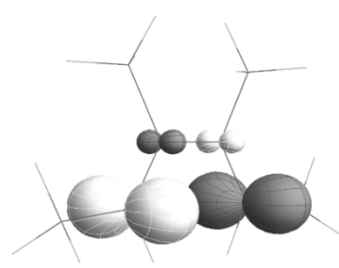
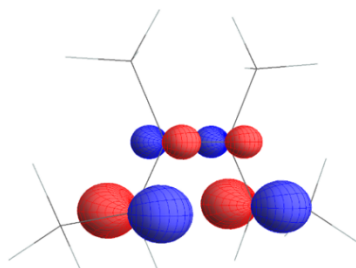
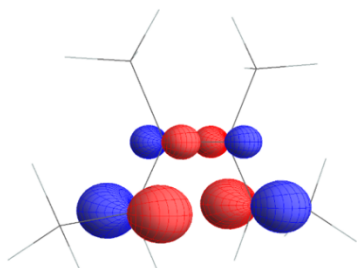
$$\pi_3^*$$

$$\alpha-0.618\beta$$

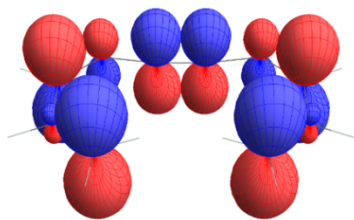


$$\pi_2 \rightarrow \pi_3^*$$

$$-1.236\beta$$

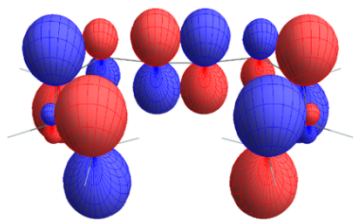


S151. Hückel HOMO and LUMO as well as corresponding overlap density for **3**



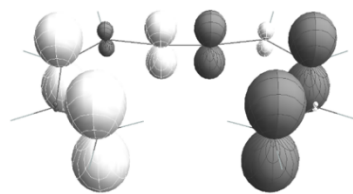
$$\pi_5$$

$$\alpha+0.285\beta$$



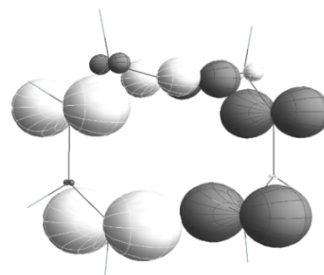
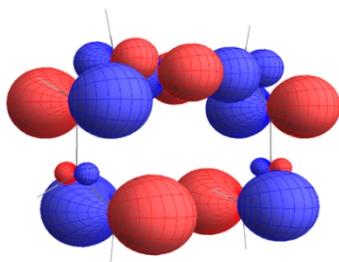
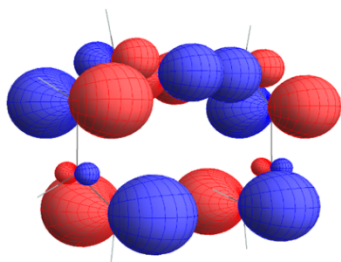
$$\pi_6^*$$

$$\alpha-0.285\beta$$

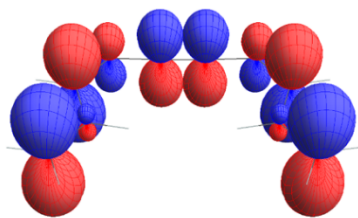


$$\pi_5 \rightarrow \pi_6^*$$

$$-0.570\beta$$

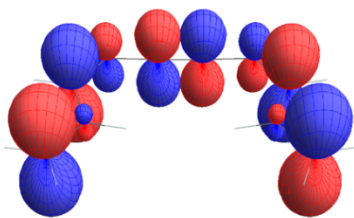


S152. Hückel HOMO and LUMO as well as corresponding overlap density for 4



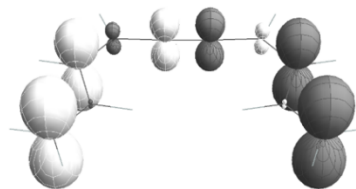
$$\pi_5$$

$$\alpha+0.285\beta$$



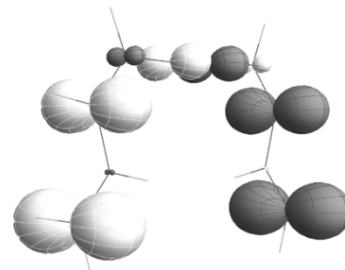
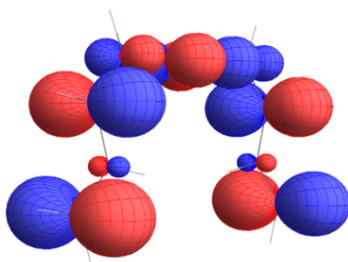
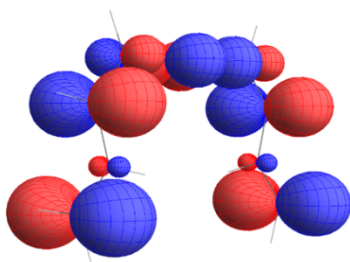
$$\pi_6^*$$

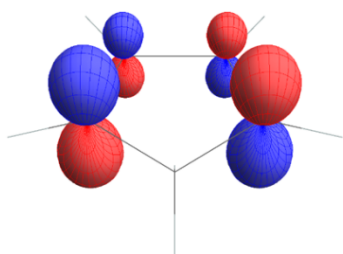
$$\alpha-0.285\beta$$



$$\pi_5 \rightarrow \pi_6^*$$

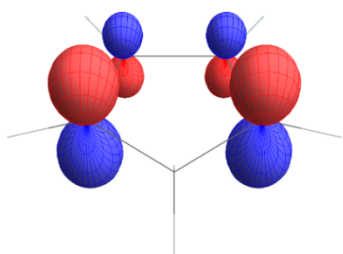
$$-0.570\beta$$





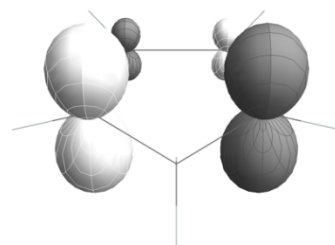
$$\pi_2$$

$$\alpha+0.618\beta$$



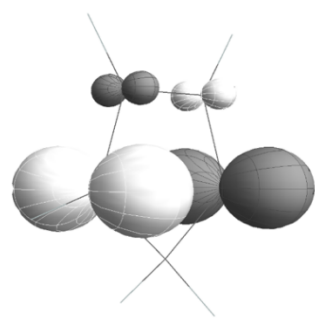
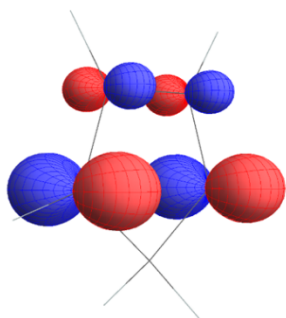
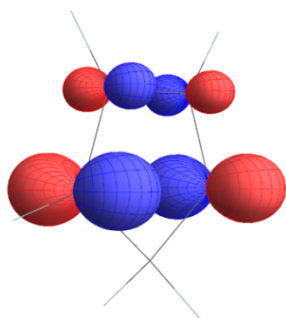
$$\pi_3^*$$

$$\alpha-0.618\beta$$

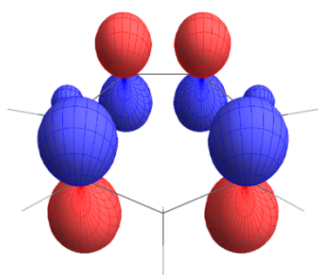


$$\pi_2 \rightarrow \pi_3^*$$

$$-1.236\beta$$

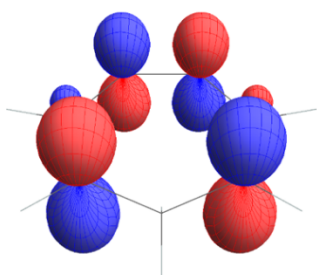


S154. Hückel HOMO and LUMO and corresponding overlap density for **6**



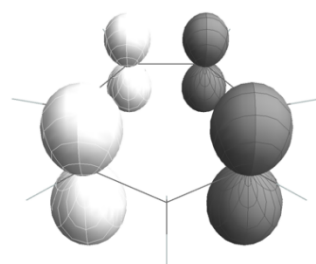
$$\pi_3$$

$$\alpha + 0.445\beta$$



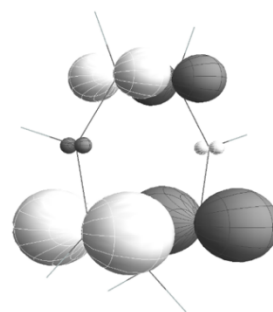
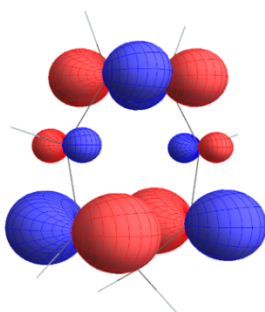
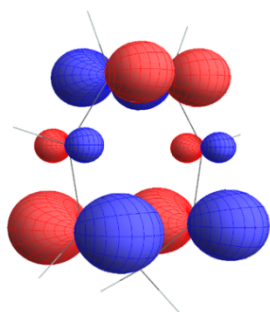
$$\pi_4^*$$

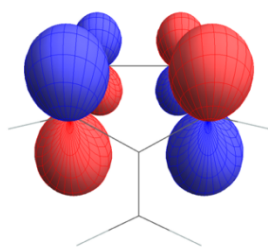
$$\alpha - 0.445\beta$$



$$\pi_3 \rightarrow \pi_4^*$$

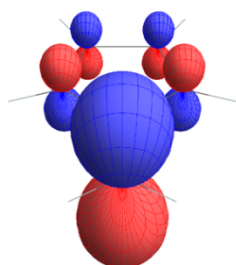
$$-0.890\beta$$





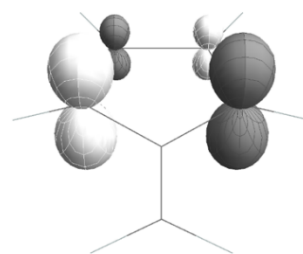
$$\pi_3$$

$$\alpha+0.618\beta$$



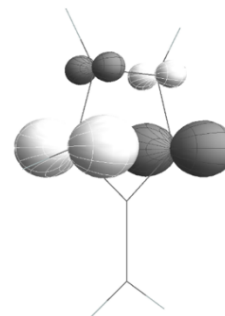
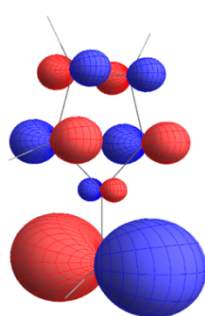
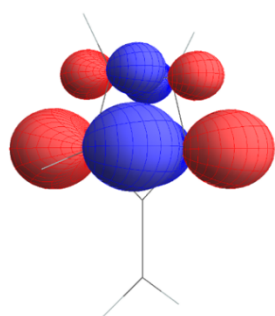
$$\pi_4^*$$

$$\alpha-0.254\beta$$

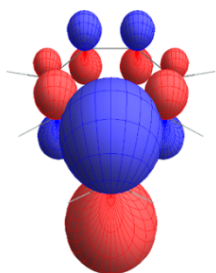


$$\pi_3 \rightarrow \pi_4^*$$

$$-0.872\beta$$

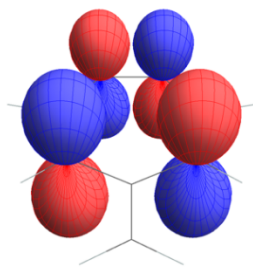


S156. Hückel HOMO and LUMO and corresponding overlap density for **8**



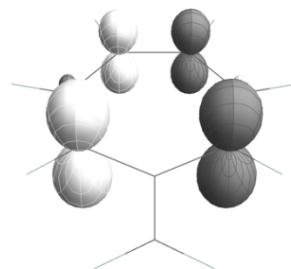
$$\pi_4$$

$$\alpha+0.216\beta$$



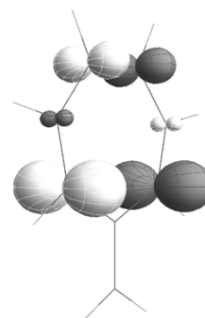
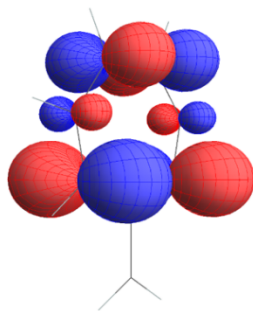
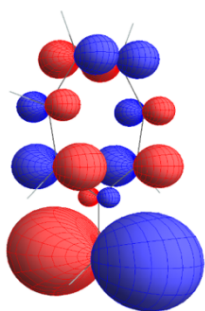
$$\pi_5^*$$

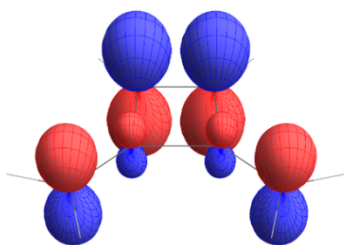
$$\alpha-0.445\beta$$



$$\pi_4 \rightarrow \pi_5^*$$

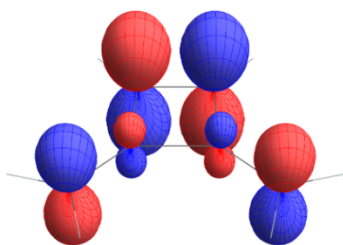
$$-0.661\beta$$





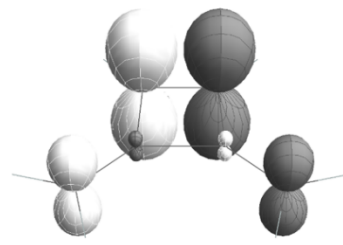
$$\pi_3$$

$$\alpha + 0.555\beta$$



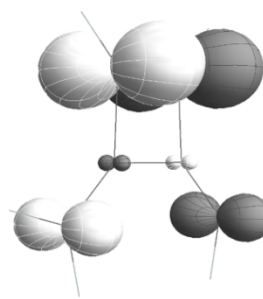
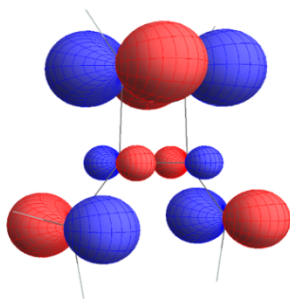
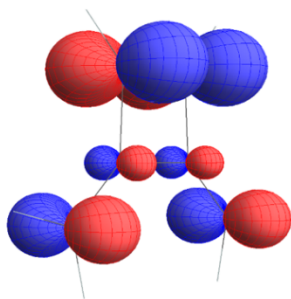
$$\pi_4^*$$

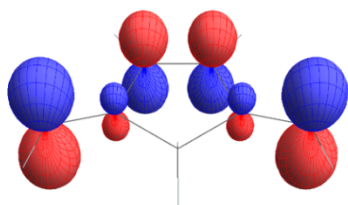
$$\alpha - 0.555\beta$$



$$\pi_3 \rightarrow \pi_4^*$$

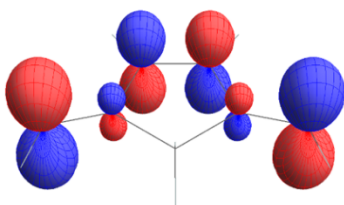
$$-1.110\beta$$





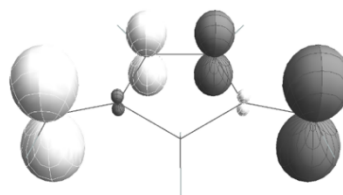
$$\pi_3$$

$$\alpha+0.445\beta$$



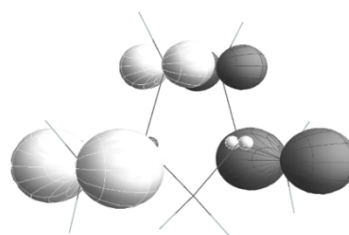
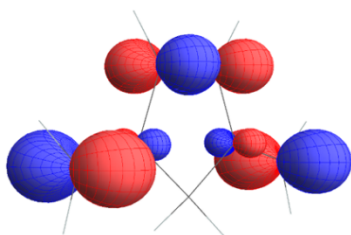
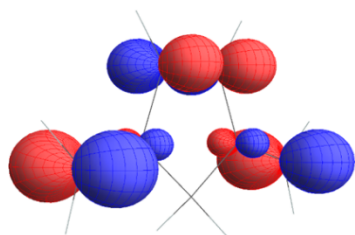
$$\pi_4^*$$

$$\alpha-0.445\beta$$

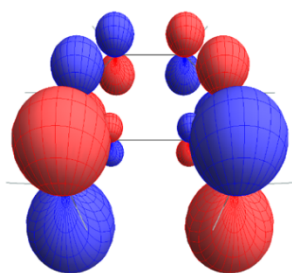


$$\pi_3 \rightarrow \pi_4^*$$

$$-0.890\beta$$

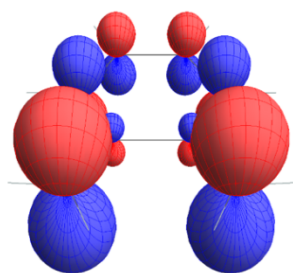


S159. *Hückel HOMO and LUMO and corresponding overlap density for 11*



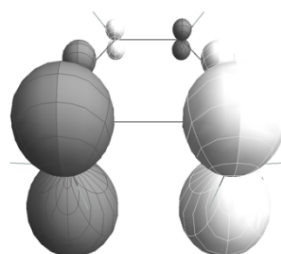
$$\pi_4$$

$$\alpha+0.295\beta$$



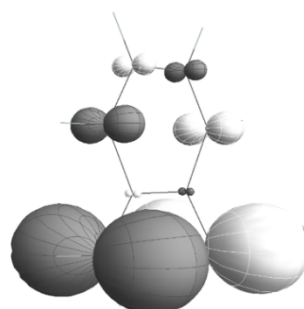
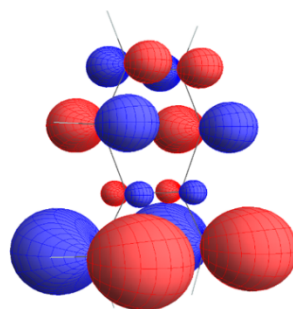
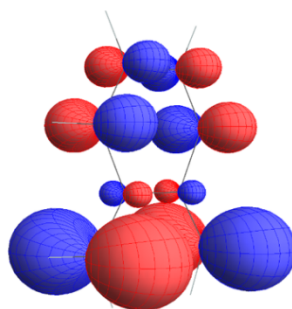
$$\pi_5^*$$

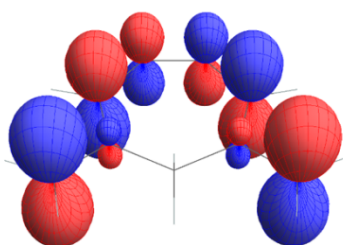
$$\alpha-0.295\beta$$



$$\pi_4 \rightarrow \pi_5^*$$

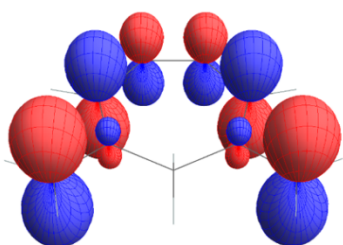
$$-0.590\beta$$





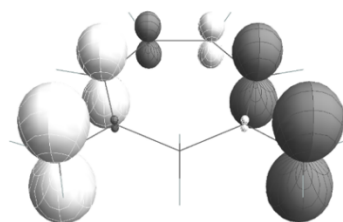
$$\pi_4$$

$$\alpha+0.347\beta$$



$$\pi_5^*$$

$$\alpha-0.347\beta$$



$$\pi_4 \rightarrow \pi_5^*$$

$$-0.694\beta$$

