A new and efficient equation-of-motion coupled-cluster framework for core-excited and core-ionized states: Supporting Information

Marta L. Vidal,[†] Xintian Feng,[‡,¶] Evgeny Epifanovsky,[¶] Anna I. Krylov,[§] and Sonia Coriani[*,†]

[†]*DTU Chemistry - Department of Chemistry, Technical University of Denmark, DK-2800, Kongens Lyngby, Denmark*

[‡]*Department of Chemistry, University of California, Berkeley, California 94720, United States*

[¶]*Q-Chem Inc., 6601 Owens Drive, Suite 105 Pleasanton, CA 94588*

[§]*Department of Chemistry, University of Southern California, Los Angeles, California 90089-0482*

E-mail: soco@kemi.dtu.dk

1 Implementation formulas of the fc-CVS-EOM-CCSD method

Notation

- I, J, ... = occupied Core orbital (very small number of orbitals - core orbitals of nuclei with different Z can be handled separately, as coupling between them is negligible)

- i_v, j_v, ... = occupied Valence orbital

- generic i, j = any occupied orbital (both core and valence)

$\mathcal{P}_+(qr)$ and $\mathcal{P}_-(qr)$ are the symmetric and antisymmetric permutation operators respectively, defined as:

$$\mathcal{P}_+(qr)f(\dots pqrs\dots) \equiv f(\dots pqrs\dots) + f(\dots prqs\dots) \tag{S1}$$

$$\mathcal{P}_-(qr)f(\dots pqrs\dots) \equiv f(\dots pqrs\dots) - f(\dots prqs\dots) \tag{S2}$$

1.1 fc-CVS-EOMEE-CCSD

1.1.1 Right transformation

$$\begin{aligned}\sigma_I^a =& \sum_b r_I^b F_{ab} - \sum_J r_J^a F_{IJ} - \sum_{Jb} r_J^b I^1_{IbJa} \\ &+ \sum_{Jb} r^{ab}_{IJ} F_{Jb} + \sum_{j_v b} r^{ab}_{Ij_v} F_{j_v b} - \sum_{Jk_v b} r^{ab}_{Jk_v} \langle Jk_v || Ib\rangle \\ &- \frac{1}{2}\sum_{JKb} r^{ab}_{JK}\langle JK||Ib\rangle - \frac{1}{2}\sum_{Jbc} r^{bc}_{IJ} I^7_{Jabc} - \frac{1}{2}\sum_{j_v bc} r^{bc}_{Ij_v} I^7_{j_v abc}\end{aligned} \tag{S3}$$

$$\begin{aligned}\sigma_{IJ}^{ab} =& -\mathcal{P}_-(ab)\sum_K I^2_{IJKb} r^a_K - \mathcal{P}_-(IJ)\sum_c I^3_{Jcab} r^c_I \\ &+ \mathcal{P}_-(IJ)\Big(\sum_K r^{ab}_{JK} F_{IK} + \sum_{k_v} r^{ab}_{Jk_v} F_{Ik_v}\Big) + \mathcal{P}_-(ab)\sum_c r^{ac}_{IJ} F_{bc} \\ &+ \mathcal{P}_-(IJ)\mathcal{P}_-(ab)\Big(\sum_{Kc} r^{ac}_{JK} I^1_{IcKb} + \sum_{k_v c} r^{ac}_{Jk_v} I^1_{Ick_v b}\Big) \\ &+ \frac{1}{2}\sum_{KL} r^{ab}_{KL}\langle IJ||KL\rangle + \sum_{Kl_v} r^{ab}_{Kl_v}\langle IJ||Kl_v\rangle + \frac{1}{2}\sum_{cd} r^{cd}_{IJ} I^5_{abcd}\end{aligned} \tag{S4}$$

$$
\begin{aligned}
\sigma^{ab}_{Ij_v} =& \mathcal{P}_-(ab)\sum_K r^a_K I^2_{j_v IKb} - \sum_c r^c_I I^3_{j_v cab} + \sum_{l_v} \tilde{T}^1_{Il_v} t^{ab}_{j_v l_v} \\
&+ \sum_K r^{ab}_{j_v K} F_{IK} - \sum_K r^{ab}_{IK} F_{j_v K} - \sum_{k_v} r^{ab}_{Ik_v} F_{j_v k_v} \\
&+ \mathcal{P}_-(ab)\sum_c r^{ac}_{Ij_v} F_{bc} - \mathcal{P}_-(ab)\sum_{k_v c} r^{ac}_{Ik_v} I^1_{j_v c k_v b} \\
&- \mathcal{P}_-(ab)\sum_{Kc} (r^{bc}_{j_v K} I^1_{IcKa} + r^{ac}_{IK} I^1_{j_v cKb}) \\
&- \frac{1}{2}\sum_{KL} r^{ab}_{KL} I^4_{j_v IKL} + \sum_{Kl_v} r^{ab}_{Kl_v} I^4_{j_v Il_v K} + \frac{1}{2}\sum_{cd} r^{cd}_{Ij_v} I^5_{abcd} + \sum_{l_v} \tilde{T}^3_{Il_v} t^{ab}_{j_v l_v}
\end{aligned}
\tag{S5}
$$

1.1.2 Left transformation

$$\begin{aligned}\tilde{\sigma}_I^a =& \sum_b l_I^b F_{ba} - \sum_J l_J^a F_{JI} - \sum_{Jb} l_J^b I^1_{JaIb} + \sum_{Jk_vb} l^{ab}_{Jk_v} I^2_{k_vJIb} \\ & - \frac{1}{2}\sum_{JKb} l^{ab}_{JK} I^2_{JKIb} - \frac{1}{2}\sum_{Jbc} l^{bc}_{IJ} I^3_{Jabc} - \frac{1}{2}\sum_{j_vbc} l^{bc}_{Ij_v} I^3_{j_vabc} - \sum_{k_vL} \tilde{T}^5_{k_vL}\langle k_vI||La\rangle \end{aligned} \tag{S6}$$

$$\begin{aligned}\tilde{\sigma}_{IJ}^{ab} =& \mathcal{P}_-(IJ)\mathcal{P}_-(ab) l_I^a F_{Jb} + \mathcal{P}_-(ab)\sum_K l_K^b \langle IJ||Ka\rangle + \mathcal{P}_-(IJ)\sum_c l_J^c I^7_{Icab} \\ & + \mathcal{P}_-(IJ)\left(\sum_K l^{ab}_{JK} F_{KI} + \sum_{k_v} l^{ab}_{Jk_v} F_{k_vI}\right) + \mathcal{P}_-(ab)\sum_c l^{ac}_{IJ} F_{cb} \\ & + \frac{1}{2}\sum_{KL} l^{ab}_{KL}\langle KL||IJ\rangle - \sum_{Kl_v} l^{ab}_{Kl_v} I^4_{l_vKIJ} + \frac{1}{2}\sum_{cd} l^{cd}_{IJ} I^5_{cdab} \\ & - \mathcal{P}_-(IJ)\mathcal{P}_-(ab)\left(\sum_{Kc} l^{ac}_{IK} I^1_{KbJc} - \sum_{k_vc} l^{ac}_{Ik_v} I^1_{k_vbJc}\right) - \mathcal{P}_-(IJ)\sum_{k_v} \tilde{T}^5_{k_vI}\langle k_vJ||ab\rangle \end{aligned} \tag{S7}$$

$$\begin{aligned}\tilde{\sigma}_{Ij_v}^{ab} =& \mathcal{P}_-(ab) l_I^a F_{j_vb} + \mathcal{P}_-(ab)\sum_K l_K^b \langle j_vI||Ka\rangle - \sum_c l_I^c I^7_{j_vcab} \\ & + \sum_K (l^{ab}_{j_vK} F_{KI} - l^{ab}_{IK} F_{Kj_v}) - \sum_{k_v} l^{ab}_{Ik_v} F_{k_vj_v} + \mathcal{P}_-(ab)\sum_c l^{ac}_{Ij_v} F_{cb} \\ & - \frac{1}{2}\sum_{KL} l^{ab}_{KL}\langle j_vI||KL\rangle + \sum_{Kl_v} l^{ab}_{Kl_v} I^4_{l_vKj_vI} + \frac{1}{2}\sum_{cd} l^{cd}_{Ij_v} I^5_{cdab} \\ & - \mathcal{P}_-(ab)\sum_{Kc}(l^{ac}_{IK} I^1_{Kbj_vc} + l^{ac}_{j_vK} I^1_{KbIc}) - \mathcal{P}_-(ab)\sum_{k_vc} l^{ac}_{Ik_v} I^1_{k_vbj_vc} \\ & + \sum_{k_v} \tilde{T}^5_{k_vI}\langle j_vk_v||ab\rangle \end{aligned} \tag{S8}$$

Table S1: Intermediates.

$F_{IJ} = f_{IJ} + \sum_{k_v a} t^a_{k_v} \langle Jk_v || Ia \rangle$
$F_{Ij_v} = f_{Ij_v} + \sum_{k_v a} t^a_{k_v} \langle j_v k_v || Ia \rangle$
$F_{i_v J} = f_{i_v J} + \sum_a t^a_{i_v} f_{Ja} + \sum_{k_v a} t^a_{k_v} \langle Jk_v || i_v a \rangle + \sum_{k_v ab} t^a_{i_v} t^b_{k_v} \langle Jk_v || ab \rangle + \frac{1}{2} \sum_{k_v bc} t^{bc}_{i_v k_v} \langle Jk_v || bc \rangle$
$F_{i_v j_v} = f_{i_v j_v} + \sum_a t^a_{i_v} f_{j_v a} + \sum_{k_v a} t^a_{k_v} \langle j_v k_v || i_v a \rangle + \sum_{k_v ab} t^a_{i_v} t^b_{k_v} \langle j_v k_v || ab \rangle + \frac{1}{2} \sum_{k_v bc} t^{bc}_{i_v k_v} \langle j_v k_v || bc \rangle$
$F_{Ia} = f_{Ia} + \sum_{j_v b} t^b_{j_v} \langle Ij_v || ab \rangle$
$F_{i_v a} = f_{i_v a} + \sum_{j_v b} t^b_{j_v} \langle i_v j_v || ab \rangle$
$F_{ab} = f_{ab} - \sum_{i_v} t^a_{i_v} f_{i_v b} + \sum_{i_v j_v c} t^c_{i_v} t^a_{j_v} \langle i_v j_v || bc \rangle$
$I^1_{IaJb} = \langle Ia || Jb \rangle - \sum_k t^b_{k_v} \langle Jk_v || Ia \rangle$
$I^1_{Iaj_v b} = \langle Ia || j_v b \rangle - \sum_k t^b_{k_v} \langle j_v k_v || Ia \rangle$
$I^1_{i_v a J b} = \langle i_v a || Jb \rangle - \sum_{k_v} t^b_{k_v} \langle Jk_v || i_v a \rangle - \sum_c t^c_{i_v} \langle Jb || ac \rangle + \sum_{k_v c} t^c_{i_v} t^b_{k_v} \langle Jk_v || ac \rangle - \sum_{k_v c} t^{bc}_{i_v k_v} \langle Jk_v || ac \rangle$
$I^1_{i_v a j_v b} = \langle i_v a || j_v b \rangle - \sum_{k_v} t^b_{k_v} \langle j_v k_v || i_v a \rangle - \sum_c t^c_{i_v} \langle j_v b || ac \rangle + \sum_{k_v c} t^c_{i_v} t^b_{k_v} \langle j_v k_v || ac \rangle - \sum_{k_v c} t^{bc}_{i_v k_v} \langle j_v k_v || ac \rangle$
$I^2_{IJKa} = \langle IJ || Ka \rangle - \sum_{l_v} t^a_{l_v} \langle IJ || K l_v \rangle$
$I^2_{i_v JKa} = \langle i_v J || Ka \rangle + \sum_{l_v} t^a_{l_v} I^4_{i_v J l_v K} - \sum_b t^b_{i_v} \langle Jb || Ka \rangle - \sum_{l_v c} t^{ac}_{i_v l_v} \langle Jc || K l_v \rangle$
$I^3_{Iabc} = \langle Ia || bc \rangle + \frac{1}{2} \sum_{j_v k_v} t^{bc}_{j_v k_v} \langle j_v k_v || Ia \rangle + \mathcal{P}_-(bc) (\sum_{j_v} t^c_{j_v} (\langle j_v b || Ia \rangle - \frac{1}{2} \sum_{k_v} t^b_{k_v} \langle j_v k_v || Ia \rangle))$
$I^3_{i_v abc} = \langle i_v a || bc \rangle - \sum_d t^d_{i_v} I^5_{bcad} + \frac{1}{2} \sum_{j_v k_v} t^{bc}_{j_v k_v} \langle j_v k_v || i_v a \rangle - \sum_{k_v} t^{bc}_{i_v k_v} (\sum_{j_v d} t^d_{j_v} \langle k_v j_v || ad \rangle) - \sum_{k_v} t^{bc}_{i_v k_v} f_{k_v a}$
$+\mathcal{P}_-(bc) (\sum_{j_v} (t^c_{j_v} (\langle j_v b || i_v a \rangle - \frac{1}{2} \sum_{k_v} t^b_{k_v} \langle j_v k_v || i_v a \rangle - \sum_{k_v d} t^{bd}_{i_v k_v} \langle j_v k_v || ad \rangle)) - \sum_{k_v d} t^{bd}_{i_v k_v} \langle k_v c || ad \rangle)$
$I^4_{i_v JKL} = \langle i_v J || KL \rangle - \sum_a t^a_{i_v} \langle KL || Ja \rangle$
$I^4_{i_v Jk_v L} = \langle i_v J || k_v L \rangle - \sum_a t^a_{i_v} \langle k_v L || Ja \rangle$
$I^5_{abcd} = \langle ab || cd \rangle + \frac{1}{2} \sum_{i_v j_v} (t^{ab}_{i_v j_v} + \mathcal{P}_-(ab) \mathcal{P}_-(ij) \frac{1}{2} t^a_{i_v} t^b_{j_v}) \langle i_v j_v || cd \rangle - \mathcal{P}_-(ab) \sum_{i_v} t^a_{i_v} \langle i_v b || cd \rangle$
$I^6_{IJk_v a} = \langle IJ || k_v a \rangle - \sum_c t^c_{k_v} \langle IJ || ac \rangle$
$I^6_{i_v Jk_v a} = \langle i_v J || k_v a \rangle - \sum_c t^c_{k_v} \langle i_v J || ac \rangle$
$I^7_{Iabc} = \langle Ia || bc \rangle - \sum_{j_v} t^a_{j_v} \langle Ij_v || bc \rangle$
$I^7_{i_v abc} = \langle i_v a || bc \rangle - \sum_{j_v} t^a_{j_v} \langle i_v j_v || bc \rangle$

$\tilde{T}^1_{Ij_v} = \sum_{Kc} r^c_K \langle j_v K || Ic \rangle$
$\tilde{T}^3_{Ij_v} = \frac{1}{2} \left(\sum_{Kcd} r^{cd}_{IK} \langle j_v K || cd \rangle + \sum_{k_v cd} r^{cd}_{Ik_v} \langle j_v k_v || cd \rangle \right)$
$\tilde{T}^5_{i_v J} = \frac{1}{2} \sum_{k_v ab} l^{ab}_{Jk_v} t^{ab}_{i_v k_v}$

$r_0 = \frac{1}{\omega} \left[\sum_{Ia} r^a_I f^a_I + \sum_{Ij_v ab} r^a_I t^b_{j_v} \langle Ij_v || ab \rangle + \frac{1}{2} \sum_{Ij_v ab} r^{ab}_{Ij_v} \langle Ij_v || ab \rangle + \frac{1}{4} \sum_{IJab} r^{ab}_{IJ} \langle IJ || ab \rangle \right]$

1.1.3 One-Electron Density Matrices

$$\gamma_{JI} = -\sum_{a} l_I^a r_J^a - \frac{1}{2}\left(\sum_{Kab} l_{IK}^{ab} r_{JK}^{ab} + \sum_{k_v ab} l_{Ik_v}^{ab} r_{Jk_v}^{ab}\right) \tag{S9}$$

$$\gamma_{j_v I} = -\frac{1}{2}\left(\sum_{Kab} r_{j_v K}^{ab} l_{IK}^{ab} + r_0 \sum_{k_v ab} t_{j_v k_v}^{ab} l_{Ik_v}^{ab}\right) - r_0 \sum_{a} t_{j_v}^{a} l_I^a - \sum_{a} t_{j_v}^{a} \sum_{Kb} r_K^b l_{IK}^{ab} \tag{S10}$$

$$\gamma_{J i_v} = -\frac{1}{2}\sum_{Kab} l_{i_v K}^{ab} r_{JK}^{ab} \tag{S11}$$

$$\gamma_{i_v j_v} = -\frac{1}{2}\sum_{Kab} l_{i_v K}^{ab} r_{j_v K}^{ab} - \sum_{a} t_{j_v}^{a} \sum_{Kb} l_{i_v K}^{ab} r_K^b \tag{S12}$$

$$\gamma_{ab} = \sum_{I} r_I^b l_I^a + \frac{1}{2}\sum_{IJc} r_{IJ}^{bc} l_{IJ}^{ac} + \sum_{Ij_v c} r_{Ij_v}^{bc} l_{Ij_v}^{ac} + \sum_{i_v} t_{i_v}^{b} \sum_{Kc} r_K^c l_{i_v K}^{ac} \tag{S13}$$

$$\gamma_{Ia} = \sum_{Jb} r_{IJ}^{ab} l_J^b - \frac{1}{2}\sum_{j_v} t_{j_v}^{a}\left(\sum_{Kbc} r_{IK}^{bc} l_{j_v K}^{bc}\right) \tag{S14}$$

$$\begin{aligned}\gamma_{i_v a} = {} & t_{i_v}^{a} + \sum_{Jb}\left(r_{i_v J}^{ab} - t_{i_v}^{b} r_J^a\right) l_J^b + \sum_{j_v b}\left[\left(t_{i_v j_v}^{ab} - t_{j_v}^{a} t_{i_v}^{b}\right)\sum_{Kc} l_{j_v K}^{bc} r_K^c\right] \\ & - \frac{1}{2}\sum_{K} r_K^a\left(\sum_{j_v bc} l_{K j_v}^{bc} t_{i_v j_v}^{bc}\right) - \frac{1}{2}\sum_{j_v} t_{j_v}^{a}\left(\sum_{Kbc} r_{i_v K}^{bc} l_{j_v K}^{bc}\right) \\ & - \sum_{b} t_{i_v}^{b}\left(\frac{1}{2}\sum_{JKc} r_{JK}^{ac} l_{JK}^{bc} + \sum_{Jk_v c} r_{Jk_v}^{ac} l_{Jk_v}^{bc}\right)\end{aligned} \tag{S15}$$

$$\gamma_{aI} = r_0 l_I^a + \sum_{Jb} r_J^b l_{IJ}^{ab} \tag{S16}$$

$$\gamma_{a i_v} = \sum_{Jb} r_J^b l_{i_v J}^{ab} \tag{S17}$$

1.2 fc-CVS-EOMIP-CCSD

1.2.1 Right transformation

$$\begin{aligned}\sigma_I =& -\sum_J F_{IJ} r_J + \sum_{Jb} F_{Jb} r^b_{IJ} + \sum_{j_v b} F_{j_v b} r^b_{Ij_v} \\ & - \frac{1}{2}\sum_{JKb} \langle JK||Ib\rangle r^b_{JK} - \sum_{Jk_v b} \langle Jk_v||Ib\rangle r^b_{Jk_v}\end{aligned} \tag{S18}$$

$$\begin{aligned}\sigma^a_{IJ} =& -\sum_K r_K I^2_{IJKa} + \sum_b r^b_{IJ} F_{ab} \\ & + \mathcal{P}_-(IJ)\left(\sum_K r^a_{JK} F_{IK} + \sum_{k_v} r^a_{Jk_v} F_{Ik_v}\right) \\ & - \mathcal{P}_-(IJ)\left(\sum_{Kb} I^1_{JbKa} r^b_{IK} + \sum_{k_v b} I^1_{Jbk_v a} r^b_{Ik_v}\right) \\ & + \frac{1}{2}\sum_{KL} \langle IJ||KL\rangle r^a_{KL} + \sum_{Kl_v} \langle IJ||Kl_v\rangle r^a_{Kl_v}\end{aligned} \tag{S19}$$

$$\begin{aligned}\sigma^a_{Ij_v} =& \sum_K r_K I^2_{j_v IKa} + \sum_b r^b_{Ij_v} F_{ab} \\ & + \sum_K r^a_{j_v K} F_{IK} - \sum_K r^a_{IK} F_{j_v K} - \sum_{k_v} r^a_{Ik_v} F_{j_v k_v} \\ & - \sum_{Kb} I^1_{j_v bKa} r^b_{IK} - \sum_{k_v b} I^1_{j_v bk_v a} r^b_{Ik_v} + \sum_{Kb} I^1_{IbKa} r^b_{j_v K} \\ & - \frac{1}{2}\sum_{KL} I^4_{j_v IKL} r^a_{KL} + \sum_{Kl_v} I^4_{j_v Il_v K} r^a_{Kl_v}\end{aligned} \tag{S20}$$

1.2.2 Left transformation

$$\tilde{\sigma}_I = -\sum_J F_{JI} l_J - \frac{1}{2}\sum_{JKb} I^2_{JKIb} l^b_{JK} + \sum_{Jk_vb} I^2_{k_vJIb} l^b_{Jk_v} \tag{S21}$$

$$\begin{aligned}\tilde{\sigma}^a_{IJ} =& \mathcal{P}_-(IJ) l_I F_{Ja} - \sum_K l_K \langle IJ||Ka\rangle + \sum_b l^b_{IJ} F_{ba} \\ &+ \mathcal{P}_-(IJ)\left(\sum_K l^a_{JK} F_{KI} + \sum_{k_v} l^a_{Jk_v} F_{k_vI}\right) \\ &+ \frac{1}{2}\sum_{KL}\langle KL||IJ\rangle l^a_{KL} - \sum_{Kl_v} I^4_{l_vKIJ} l^a_{Kl_v} \\ &- \mathcal{P}_-(IJ)\left(\sum_{Kb} I^1_{KaJb} l^b_{IK} + \sum_{k_vb} I^1_{k_vaJb} l^b_{Ik_v}\right)\end{aligned} \tag{S22}$$

$$\begin{aligned}\tilde{\sigma}^a_{Ij_v} =& l_I F_{j_va} - \sum_K l_K \langle Ij_v||Ka\rangle + \sum_b l^b_{Ij_v} F_{ba} \\ &+ \sum_K l^a_{j_vK} F_{KI} - \sum_K l^a_{IK} F_{Kj_v} - \sum_{k_v} l^a_{Ik_v} F_{k_vj_v} \\ &+ \frac{1}{2}\sum_{KL}\langle KL||Ij_v\rangle l^a_{KL} + \sum_{Kl_v} I^4_{l_vKj_vI} l^a_{Kl_v} \\ &- \sum_{Kb} I^1_{Kaj_vb} l^b_{IK} - \sum_{k_vb} I^1_{k_vaj_vb} l^b_{Ik_v} + \sum_{Kb} I^1_{KaIb} l^b_{j_vK}\end{aligned} \tag{S23}$$

1.2.3 One-electron Density Matrices

$$\gamma_{JI} = -l_I r_J - \sum_{Ka} l^a_{IK} r^a_{JK} - \sum_{k_v a} l^a_{Ik_v} r^a_{Jk_v} \tag{S24}$$

$$\gamma_{Ji_v} = -\sum_{Ka} l^a_{i_v K} r^a_{JK} \tag{S25}$$

$$\gamma_{j_v I} = -\sum_{Ka} l^a_{IK} r^a_{j_v K} + \sum_a t^a_{j_v} \sum_K l^a_{IK} r_K \tag{S26}$$

$$\gamma_{j_v i_v} = -\sum_{Ka} l^a_{i_v K} r^a_{j_v K} + \sum_a t^a_{j_v} \sum_K l^a_{i_v K} r_K \tag{S27}$$

$$\gamma_{ab} = \frac{1}{2} \sum_{IJ} l^a_{IJ} r^b_{IJ} + \sum_{Ij_v} l^a_{Ij_v} r^b_{Ij_v} - \sum_{i_v} t^b_{i_v} \sum_K l^a_{i_v K} r_K \tag{S28}$$

$$\gamma_{Ia} = \sum_J r^a_{JI} l_J - \sum_{j_v} t^a_{j_v} \sum_{Ka} l^a_{j_v K} r^a_{IK} \tag{S29}$$

$$\begin{aligned} \gamma_{i_v a} = \;& t^a_{i_v} - \sum_J r^a_{i_v J} l_J - \sum_{j_v b} \left[\left(t^{ab}_{i_v j_v} - t^a_{j_v} t^b_{i_v} \right) \sum_K l^b_{j_v K} r_K \right] \\ & - \sum_{j_v} t^a_{j_v} \sum_{Kb} l^b_{j_v K} r^b_{i_v K} - \sum_b t^b_{i_v} \left(\frac{1}{2} \sum_{JK} l^b_{JK} r^a_{JK} + \sum_{Jk_v} l^b_{Jk_v} r^a_{Jk_v} \right) \end{aligned} \tag{S30}$$

$$\gamma_{aI} = -\sum_J l^a_{IJ} r_J \tag{S31}$$

$$\gamma_{ai_v} = -\sum_J l^a_{i_v J} r_J \tag{S32}$$

$$\tag{S33}$$

2 Tables of computed energies, oscillator strengths and ionization energies

Table S2: Neon. fc-CVS-EOM-CCSD core excitation energies (EE) ω_i (eV), oscillator strengths f, and ionization energies (IE, eV) with different basis sets.

	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg			aug-cc-pCVTZ + Rydberg			Exp.
	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	ω_i
EE	B_{nu}	867.94	0.01063	B_{nu}	867.53	0.01180	B_{nu}	866.91	0.01190	867.12 ($\pm$ 0.05)[?]
	B_{nu}	869.55	0.00311	B_{nu}	869.20	0.00347	B_{nu}	868.57	0.00349	868.69 ($\pm$ 0.04)[?]
	B_{nu}	870.13	0.00133	B_{nu}	869.79	0.00150	B_{nu}	869.17	0.00151	869.27 ($\pm$ 0.05)[?]
IE	A_g	870.91		A_g	870.58		A_g	869.96		870.17[?]

Table S3: Water. fc-CVS-EOM-CCSD O-edge excitation energies (EE) ω_i (eV), oscillator strengths f, and ionization energies (IE, eV) with different basis sets.

	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	ω_i
	6-311++G**			aug-cc-pVTZ			aug-cc-pCVTZ			Exp.[?]
EE	A_1	535.22	0.01277	A_1	534.86	0.01273	A_1	534.43	0.01289	534.0[?]
	B_1	537.01	0.02651	B_1	536.65	0.02603	B_1	536.22	0.02644	535.9[?]
	A_1	539.73	0.01821	A_1	538.46	0.01169	A_1	538.03	0.01174	
	B_2	539.93	0.02018	B_2	538.55	0.01513	B_2	538.12	0.01524	
	B_1	540.08	0.01133	B_1	539.22	0.01020	B_1	538.79	0.01009	
	A_1	540.55	0.00074	A_1	539.23	0.00014	A_1	538.81	0.00014	
	B_1	542.39	0.00831	B_1	540.67	0.00104	B_1	540.25	0.00101	
	A_1	542.55	0.00010	A_1	540.86	0.00013	A_1	540.44	0.00013	
	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg			aug-cc-pCVTZ + Rydberg			Exp.
EE	A_1	535.21	0.01288	A_1	534.86	0.01277	A_1	534.42	0.01294	534.0[?]
	B_1	537.00	0.02604	B_1	536.65	0.02602	B_1	536.21	0.02643	535.9[?]
	B_2	538.20	0.00670	B_2	537.89	0.00779	B_2	537.47	0.00791	
	A_1	538.32	0.00399	A_1	537.97	0.00502	A_1	537.55	0.00509	
	A_1	538.84	0.00247	A_1	538.51	0.00212	A_1	538.09	0.00210	
	B_1	539.14	0.00415	B_1	538.79	0.00418	B_1	538.37	0.00421	
	A_1	539.41	0.00002	A_1	539.08	0.00001	A_1	538.66	0.00001	
	B_1	539.52	0.00132	B_1	539.18	0.00125	B_1	538.76	0.00123	
	A_1	539.54	0.00002	A_1	539.21	0.00000	A_1	538.80	0.00000	
	B_2	539.55	0.00005	B_2	539.22	0.00003	B_2	538.80	0.00003	
	B_2	539.69	0.00184	B_2	539.37	0.00240	B_2	538.95	0.00243	
	A_1	539.73	0.00125	A_1	539.40	0.00171	A_1	538.98	0.00172	
	A_1	539.89	0.00091	A_1	539.56	0.00068	A_1	539.14	0.00066	
	B_1	539.99	0.00124	B_1	539.65	0.00132	B_1	539.23	0.00132	
	A_1	540.11	0.00001	A_1	539.79	0.00000	A_1	539.37	0.00000	
	B_1	540.16	0.00062	B_1	539.85	0.00056	B_1	539.43	0.00056	
	A_1	540.17	0.00001	A_1	539.87	0.00000	A_1	539.45	0.00000	
	B_2	540.17	0.00003	B_2	539.87	0.00000	B_2	539.45	0.00000	
	B_2	540.24	0.00080	B_2	539.92	0.00125	B_2	539.50	0.00127	
	A_1	540.27	0.00096	A_1	539.93	0.00098	A_1	539.51	0.00097	
	B_1	540.38	0.00064	B_1	540.11	0.00112	B_1	539.70	0.00111	
	B_2	540.52	0.00000	B_2	540.44	0.00001	B_2	540.03	0.00001	
	B_1	540.52	0.00043	B_1	540.45	0.00115	B_1	540.03	0.00114	
	B_2	540.57	0.00082	B_2	540.81	0.00703	B_2	540.38	0.00701	
	B_1	540.75	0.00129	B_1	541.14	0.00353	B_1	540.72	0.00348	
IE	A_1	540.99		A_1	540.65		A_1	540.23		539.9[?]

Table S4: Ammonia. fc-CVS-EOMEE-CCSD N-edge excitation energies (EE) ω_i (eV), oscillator strengths f, and core ionization energies (IE, eV).

	Symm.	ω_i	f	Symm.	ω_i	f
	6-311++G**			aug-cc-pVTZ		
EE	A_1	401.57	0.00630	A_1	401.21	0.00626
	E	403.28	0.04205	E	402.87	0.04040
	A_1	404.88	0.01667	A_1	404.00	0.01238
	E	405.68	0.01633	E	404.85	0.02109
	A_1	406.32	0.00068	A_1	404.89	0.00062
				A_1	405.66	0.00662
	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg		
EE	A_1	401.57	0.00635	A_1	401.20	0.00631
	E	403.23	0.03859	E	402.86	0.03995
	A_1	403.89	0.00556	A_1	403.51	0.00629
	A_1	404.55	0.00155	E	404.17	0.00730
	E	404.57	0.00800	A_1	404.21	0.00148
	E	404.95	0.00020	E	404.56	0.00047
	A_1	404.98	0.00003	A_1	404.62	0.00001
	E	405.06	0.00572	E	404.72	0.00586
	A_1	405.22	0.00158	A_1	404.88	0.00178
	E	405.42	0.00246	E	405.07	0.00207
	A_1	405.44	0.00062	A_1	405.11	0.00059
	A_1	405.61	0.00001	E	405.24	0.00014
	E	405.61	0.00004	A_1	405.27	0.00000
	E	405.66	0.00239	E	405.32	0.00247
	A_1	405.73	0.00071	A_1	405.39	0.00081
	E	405.82	0.00135	E	405.48	0.00109
	A_1	405.83	0.00028	A_1	405.49	0.00025
	A_1	405.96	0.00000	E	405.60	0.00018
	E	405.96	0.00013	A_1	405.61	0.00000
	E	406.00	0.00152	E	405.66	0.00169
	A_1	406.04	0.00090	A_1	405.70	0.00105
	A_1	406.09	0.00009	A_1	405.76	0.00008
	A_1	406.22	0.00157	A_1	405.87	0.00135
IE	A_1	406.44		A_1	406.12	

Table S5: Carbon monoxide. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at the C edge.

C-edge	Symm.	ω_i	f	ω_i	f	
	6-311++G**+Rydberg			aug-cc-pVTZ+Rydberg		
EE	E_1	287.80	0.16144	E_1	287.25	0.16124
	A_1	293.35	0.00372	A_1	292.97	0.00380
	E_1	294.32	0.00923	E_1	293.95	0.00952
	A_1	294.46	0.00034	A_1	294.09	0.00033
	A_1	295.33	0.00024	A_1	294.97	0.00021
	A_1	295.52	0.00000	E_1	295.13	0.00000
	E_1	295.56	0.00086	E_1	295.21	0.00088
	A_1	295.57	0.00062	A_1	295.22	0.00068
	E_1	295.76	0.00280	E_1	295.41	0.00286
	A_1	295.81	0.00006	A_1	295.46	0.00006
	A_1	296.10	0.00009	A_1	295.74	0.00008
	A_1	296.18	0.00000	E_1	295.81	0.00000
	E_1	296.20	0.00042	E_1	295.86	0.00044
	A_1	296.21	0.00028	A_1	295.86	0.00030
	E_1	296.29	0.00125	E_1	295.94	0.00126
	A_1	296.31	0.00002	A_1	295.96	0.00002
	A_1	296.45	0.00008	A_1	296.10	0.00009
	E_1	296.54	0.00011	E_1	296.17	0.00000
	E_1	296.56	0.00030	A_1	296.19	0.00015
	E_1	296.61	0.00152	E_1	296.22	0.00036
	A_1	296.63	0.00000	E_1	296.26	0.00152
	A_1	296.72	0.00032	A_1	296.28	0.00000
	A_1	297.04	0.00002	A_1	296.37	0.00029
				A_1	296.68	0.00002
IE	A_1	297.03		A_1	296.68	

Table S6: Carbon monoxide. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at the O edge.

O-edge	Symm.	ω_i	f	ω_i	f	
	6-311++G**+Rydberg			aug-cc-pVTZ+Rydberg		
EE	E_1	535.50	0.08163	E_1	535.01	0.08084
	A_1	540.11	0.00108	A_1	539.69	0.00104
	E_1	541.19	0.00088	E_1	540.79	0.00102
	A_1	541.37	0.00000	A_1	540.98	0.00000
	A_1	542.10	0.00015	A_1	541.70	0.00018
	A_1	542.29	0.00000	E_1	541.86	0.00000
	E_1	542.35	0.00130	E_1	541.96	0.00144
	A_1	542.36	0.00053	A_1	541.97	0.00054
	E_1	542.57	0.00030	E_1	542.18	0.00035
	A_1	542.63	0.00000	A_1	542.25	0.00000
	A_1	542.87	0.00012	A_1	542.48	0.00015
	A_1	542.96	0.00000	E_1	542.55	0.00000
	A_1	542.99	0.00024	A_1	542.61	0.00025
	E_1	542.99	0.00064	E_1	542.61	0.00071
	E_1	543.08	0.00014	E_1	542.70	0.00019
	A_1	543.11	0.00000	A_1	542.73	0.00000
	A_1	543.23	0.00005	A_1	542.85	0.00008
	A_1	543.32	0.00000	E_1	542.91	0.00000
	A_1	543.33	0.00029	A_1	542.95	0.00032
	E_1	543.35	0.00074	A_1	542.97	0.00049
IE	A_1	543.81			543.43	

Table S7: Ethylene. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV).

	Symm.	ω_i	f	Symm.	ω_i	f
	6-311++G**			aug-cc-pVTZ		
EE	B_{1u}	285.56	0.09854	B_{1u}	285.09	0.09852
	B_{3u}	288.04	0.00952	B_{3u}	287.67	0.00913
	B_{2u}	288.75	0.02927	B_{2u}	288.36	0.02810
	B_{3u}	289.07	0.00048	B_{3u}	288.67	0.00052
	B_{1u}	289.79	0.01323	B_{1u}	289.16	0.01057
	B_{2u}	290.24	0.00432	B_{3u}	289.75	0.00013
	B_{3u}	290.40	0.00101	B_{2u}	289.77	0.00467
	B_{3u}	291.02	0.00548	B_{3u}	290.33	0.01348
	B_{1u}	291.48	0.01120	B_{1u}	290.59	0.00716
				B_{2u}	290.59	0.02589
				B_{3u}	290.74	0.00001
	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg		
EE	B_{1u}	285.55	0.09851	B_{1u}	285.09	0.09864
	B_{3u}	288.00	0.00882	B_{3u}	287.67	0.00909
	B_{2u}	288.68	0.02583	B_{2u}	288.35	0.02749
	B_{3u}	288.96	0.00051	B_{3u}	288.65	0.00054
	B_{1u}	289.20	0.00555	B_{1u}	288.88	0.00623
	B_{3u}	289.70	0.00053	B_{3u}	289.35	0.00060
	B_{3u}	289.92	0.00196	B_{3u}	289.61	0.00215
	B_{2u}	289.93	0.00440	B_{2u}	289.64	0.00476
	B_{3u}	290.05	0.00159	B_{3u}	289.76	0.00173
	B_{1u}	290.11	0.00202	B_{1u}	289.82	0.00214
	B_{2u}	290.21	0.00746	B_{2u}	289.91	0.00754
	B_{3u}	290.32	0.00025	B_{3u}	290.03	0.00024
	B_{1u}	290.39	0.00198	B_{1u}	290.09	0.00214
	B_{3u}	290.52	0.00039	B_{3u}	290.21	0.00044
	B_{3u}	290.61	0.00080	B_{3u}	290.32	0.00083
	B_{2u}	290.63	0.00184	B_{2u}	290.34	0.00207
	B_{3u}	290.69	0.00066	B_{3u}	290.40	0.00071
	B_{1u}	290.71	0.00088	B_{1u}	290.42	0.00093
	B_{2u}	290.76	0.00381	B_{2u}	290.46	0.00363
	B_{3u}	290.84	0.00059	B_{3u}	290.55	0.00059
	B_{1u}	290.85	0.00100	B_{1u}	290.57	0.00107
	B_{2u}	290.99	0.00225	B_{2u}	290.69	0.00215
	B_{1u}	291.07	0.00115	B_{2u}	290.76	0.00033
	B_{2u}	291.07	0.00206	B_{1u}	290.78	0.00121
	B_{1u}	291.18	0.00095	B_{1u}	290.90	0.00096
	B_{2u}	291.41	0.00490	B_{2u}	290.91	0.00031
IE	B_{3u}	291.49		B_{3u}	291.21	

Table S8: Vinylfluoride. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization potentials (IE, eV).

	Symm.	ω_i	f	Symm.	ω_i	f
	6-311++G**			aug-cc-pVTZ		
EE	A”	285.91	0.04591	A”	285.44	0.04569
	A”	288.04	0.05894	A”	287.55	0.05877
	A’	288.18	0.00586	A’	287.80	0.00551
	A’	288.81	0.01206	A’	288.40	0.01197
	A’	289.52	0.00432	A’	289.03	0.00353
	A”	289.85	0.00817	A”	289.22	0.00664
	A’	289.88	0.00287	A’	289.37	0.00375
	A’	290.63	0.01805	A’	290.00	0.00062
	A’	290.64	0.00311	A’	290.23	0.02172
	A’	291.13	0.00480	A’	290.38	0.00855
	A’	291.48	0.02197	A”	290.68	0.00356
	A”	291.52	0.00531	A’	290.76	0.00036
	A’	291.66	0.00151	A’	290.84	0.00548
	A’	291.83	0.00870	A’	290.99	0.01957
	A’	292.07	0.01011	A’	291.23	0.00239
	A’	292.34	0.00263	A’	291.35	0.00379
	A”	292.47	0.00326	A’	291.66	0.00003
	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg		
EE	A”	285.90	0.04582	A”	285.44	0.04578
	A”	288.03	0.05889	A”	287.55	0.05888
	A’	288.15	0.00537	A’	287.79	0.00549
	A’	288.76	0.01100	A’	288.40	0.01179
	A”	289.33	0.00411	A’	288.97	0.00298
	A’	289.34	0.00303	A”	288.97	0.00435
	A’	289.69	0.00433	A’	289.26	0.00404
	A’	290.06	0.00156	A’	289.70	0.00161
	A’	290.17	0.00114	A’	289.81	0.00123
	A’	290.31	0.00027	A”	289.96	0.00049
	A”	290.33	0.00068	A’	289.97	0.00034
	A”	290.41	0.00034	A”	290.05	0.00071
	A’	290.44	0.00120	A’	290.11	0.00122
	A’	290.58	0.00128	A’	290.23	0.02274
	A”	290.58	0.00128	A’	290.24	0.00023
	A’	290.61	0.01916	A”	290.25	0.00132
	A’	290.68	0.00105	A’	290.33	0.00093
	A’	290.80	0.00092	A’	290.46	0.00092
	A’	290.86	0.00029	A’	290.53	0.00033
	A’	290.94	0.00013	A”	290.60	0.00016
	A”	290.95	0.00027	A’	290.61	0.00017
	A”	290.98	0.00020	A”	290.65	0.00040
	A’	291.00	0.00058	A’	290.67	0.00061
	A’	291.06	0.00033	A’	290.73	0.00034
	A”	291.06	0.00058	A”	290.74	0.00063
	A’	291.11	0.00042	A’	290.78	0.00037
	A’	291.16	0.00055	A’	290.83	0.00052
	A’	291.22	0.00022	A’	290.89	0.00026
	A’	291.26	0.00019	A’	290.93	0.00024
	A”	291.31	0.00016	A”	290.95	0.00006
	A’	291.32	0.00027	A’	290.97	0.01853
	A”	291.34	0.00067	A’	290.99	0.00019
	A’	291.38	0.00056	A”	291.01	0.00090
	A”	291.40	0.00032	A’	291.04	0.00053
	A’	291.43	0.01864	A”	291.08	0.00052
	A’	291.45	0.00037	A’	291.12	0.00038
	A’	291.51	0.00069	A’	291.15	0.00026
	A’	291.55	0.00309	A’	291.17	0.00027
	A’	291.59	0.00083	A’	291.21	0.00284
	A’	291.73	0.00099	A’	291.25	0.00088
	A’	291.88	0.00055	A’	291.38	0.00082
	A’	291.93	0.00105	A’	291.39	0.00109
	A”	291.93	0.00269	A”	291.48	0.00032
IE	A’ (C_{CH_2})	291.77		A’ (C_{CH_2})	291.44	
	A’ (C_{CHF})	294.31		A’ (C_{CHF})	294.00	

Table S9: Vinylfluoride, CH_2CHF. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at the Fluorine edge.

	Symm.	ω_i	f	Symm.	ω_i	f
	6-311++G**			aug-cc-pVTZ		
EE	A'	691.18	0.01034	A"	690.78	0.00901
	A"	691.28	0.00911	A'	690.78	0.00940
	A'	692.25	0.01700	A'	691.85	0.01791
	A'	692.70	0.00207	A'	692.23	0.00214
	A'	693.18	0.00695	A'	692.66	0.00611
	A"	693.49	0.00104	A"	692.77	0.00102
	A'	694.36	0.00249	A'	693.63	0.00188
	A'	694.71	0.00992	A'	693.80	0.00472
	A'	695.10	0.00066	A'	694.34	0.00097
	A"	695.56	0.00002	A"	694.46	0.00003
	A'	695.72	0.00019	A'	694.51	0.00230
	A'	696.29	0.00009	A'	694.82	0.00148
	6-311++G** + Rydberg			aug-cc-pVTZ + Rydberg		
EE	A'	691.14	0.00890	A"	690.77	0.00897
	A"	691.27	0.00901	A'	690.77	0.00907
	A'	692.17	0.01860	A'	691.82	0.01863
	A'	692.49	0.00210	A'	692.16	0.00195
	A"	692.70	0.00078	A"	692.37	0.00084
	A'	692.82	0.00450	A'	692.50	0.00431
	A'	693.49	0.00078	A'	693.17	0.00085
	A'	693.54	0.00023	A'	693.22	0.00029
	A'	693.60	0.00006	A"	693.27	0.00064
	A"	693.60	0.00046	A'	693.28	0.00007
	A'	693.71	0.00286	A'	693.40	0.00277
	A"	693.75	0.00005	A"	693.44	0.00003
	A'	693.84	0.00026	A'	693.53	0.00025
	A"	693.91	0.00027	A"	693.60	0.00028
	A'	693.95	0.00084	A'	693.65	0.00082
	A'	694.19	0.00036	A'	693.88	0.00040
	A'	694.21	0.00019	A'	693.90	0.00021
	A'	694.24	0.00004	A"	693.92	0.00031
	A"	694.24	0.00024	A'	693.93	0.00004
	A'	694.29	0.00090	A'	693.98	0.00084
	A"	694.31	0.00001	A"	694.00	0.00000
	A'	694.35	0.00009	A'	694.04	0.00009
	A"	694.38	0.00012	A"	694.07	0.00013
	A'	694.40	0.00036	A'	694.10	0.00034
	A'	694.52	0.00025	A'	694.22	0.00026
	A'	694.57	0.00027	A'	694.25	0.00025
	A'	694.59	0.00008	A'	694.28	0.00012
	A"	694.59	0.00027	A"	694.28	0.00031
	A'	694.62	0.00048	A'	694.31	0.00034
	A"	694.66	0.00000	A"	694.35	0.00001
	A'	694.68	0.00002	A'	694.37	0.00002
	A"	694.72	0.00011	A"	694.42	0.00009
	A'	694.73	0.00065	A'	694.42	0.00065
	A'	694.82	0.00020	A'	694.49	0.00027
	A'	695.09	0.00075	A'	694.53	0.00003
	A'	695.11	0.00028	A'	694.63	0.00034
	A'	695.15	0.00013	A'	694.78	0.00048
	A"	695.17	0.00066	A'	694.81	0.00040
	A"	695.32	0.00001	A"	694.82	0.00076
IE	A'	695.07		A'	694.77	

Table S10: Ozone. fc-CVS-EOM-CCSD core excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV).

	Symm.	ω_i	f	Symm.	ω_i	f
	6-311++G**			aug-cc-pVTZ		
EE	B_2	531.55	0.08818	B_2	531.16	0.08714
	B_2	536.11	0.04986	B_2	535.62	0.05113
	B_1	537.78	0.10280	B_1	537.36	0.10157
	A_1	537.79	0.02705	A_1	537.37	0.02678
	A_1	541.60	0.00001	A_1	540.65	0.00000
	B_1	541.60	0.00185	B_1	540.65	0.00260
	B_1	542.23	0.00019	B_1	541.31	0.00049
	A_1	542.23	0.01996	A_1	541.31	0.01587
	B_2	542.89	0.01368	B_2	541.60	0.01013
	B_1	543.20	0.00204	B_1	541.64	0.00289
	A_1	543.20	0.00963	A_1	541.64	0.00515
	A_1	543.90	0.00006	B_1	542.68	0.00964
	B_1	543.90	0.01828	A_1	542.69	0.00026
	B_2	545.32	0.00713	B_2	543.59	0.00450
	B_2	546.20	0.00025	B_2	544.08	0.00007

	6-311++G**+Rydberg			aug-cc-pVTZ+Rydberg		
EE	B_2	531.55	0.08811	B_2	531.16	0.08711
	B_2	536.11	0.04988	B_2	535.62	0.05112
	A_1	537.78	0.02696	B_1	537.36	0.10163
	B_1	537.78	0.10251	A_1	537.37	0.02678
	A_1	540.33	0.00051	A_1	539.90	0.00047
	B_1	540.33	0.00100	B_1	539.91	0.00108
	B_2	541.25	0.00405	B_2	540.85	0.00423
	B_1	541.27	0.00071	B_1	540.86	0.00078
	A_1	541.27	0.00937	A_1	540.86	0.00959
	A_1	541.44	0.00056	A_1	541.03	0.00062
	B_1	541.44	0.00227	B_1	541.03	0.00233
	A_1	542.25	0.00038	A_1	541.83	0.00047
	B_1	542.25	0.00098	B_1	541.84	0.00111
	A_1	542.37	0.00003	A_1	541.97	0.00005
	B_1	542.37	0.00033	B_1	541.97	0.00038
	B_2	542.41	0.00066	B_2	542.01	0.00073
	B_1	542.44	0.00001	B_1	542.05	0.00003
	A_1	542.44	0.00002	A_1	542.05	0.00006
	B_2	542.44	0.00004	B_2	542.05	0.00006
	A_1	542.46	0.00102	B_1	542.07	0.00091
	B_1	542.47	0.00091	A_1	542.07	0.00107
	B_1	542.60	0.00030	B_1	542.21	0.00035
	A_1	542.60	0.00402	A_1	542.21	0.00403
	B_2	542.64	0.00118	B_2	542.26	0.00122
	A_1	542.71	0.00021	A_1	542.31	0.00023
	B_1	542.71	0.00031	B_1	542.32	0.00030
	A_1	542.95	0.00091	A_1	542.55	0.00089
	B_1	542.95	0.00111	B_1	542.55	0.00117
	B_1	543.03	0.00005	B_1	542.64	0.00006
	A_1	543.03	0.00008	A_1	542.64	0.00009
	B_2	543.06	0.00029	B_2	542.67	0.00030
	A_1	543.07	0.00000	A_1	542.69	0.00001
	B_1	543.07	0.00001	B_1	542.69	0.00002
	B_2	543.08	0.00007	B_2	542.69	0.00010
	B_1	543.09	0.00022	B_1	542.70	0.00020
	A_1	543.09	0.00079	A_1	542.70	0.00081
	B_1	543.13	0.00025	B_1	542.74	0.00029
	A_1	543.13	0.00147	A_1	542.74	0.00142
	B_2	543.16	0.00051	B_2	542.78	0.00053
	B_1	543.19	0.00009	B_1	542.81	0.00008
	A_1	543.19	0.00012	A_1	542.81	0.00014
	A_1	543.30	0.00067	A_1	542.91	0.00056
	B_1	543.30	0.00078	B_1	542.91	0.00076
	B_1	543.36	0.00003	B_1	542.97	0.00004
	A_1	543.36	0.00026	A_1	542.97	0.00024
	B_1	543.42	0.00003	B_1	543.03	0.00004
	A_1	543.42	0.00013	A_1	543.03	0.00015
	B_2	543.42	0.00029	B_2	543.03	0.00026
	B_1	543.43	0.00000	B_1	543.04	0.00000
	A_1	543.43	0.00073	B_2	543.05	0.00025
	B_2	543.44	0.00017	A_1	543.05	0.00072
	A_1	543.47	0.00046	A_1	543.08	0.00039
	B_1	543.47	0.00061	B_1	543.08	0.00063
	B_2	543.50	0.00044	B_2	543.11	0.00040
	B_1	543.53	0.00010	B_1	543.14	0.00011
	A_1	543.53	0.00021	A_1	543.14	0.00017
	B_1	543.60	0.00001	B_1	543.21	0.00000
	A_1	543.60	0.00023	A_1	543.21	0.00020
	B_1	543.67	0.00090	B_1	543.28	0.00084
	A_1	543.67	0.00118	A_1	543.28	0.00099
	B_1	543.99	0.00001	B_1	543.59	0.00001
	A_1	543.99	0.00150	A_1	543.59	0.00154
IE	A_1	543.91		A_1	543.52	
	A_1	549.03		A_1	548.67	

Table S11: Adenine. C and N CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at two different geometries.

	C-edge						N-edge					
	non-planar			planar			non-planar			planar		
	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f
EE	A	287.50	0.0616	A”	287.54	0.0619	A	400.83	0.0435	A”	400.85	0.0440
	A	287.90	0.0461	A”	287.94	0.0255	A	400.94	0.0422	A”	400.97	0.0415
	A	287.92	0.0509	A”	287.95	0.0715	A	401.10	0.0454	A”	401.14	0.0450
	A	288.12	0.0007	A”	288.16	0.0011	A	401.98	0.0000	A”	402.00	0.0000
	A	288.28	0.0718	A”	288.42	0.0701	A	402.93	0.0018	A”	402.86	0.0021
	A	288.55	0.0644	A”	288.56	0.0661	A	403.08	0.0055	A’	403.12	0.0055
	A	289.26	0.0004	A’	289.24	0.0004	A	403.26	0.0009	A’	403.21	0.0009
	A	289.68	0.0053	A”	289.74	0.0054	A	403.39	0.0007	A’	403.30	0.0008
	A	289.81	0.0007	A’	289.78	0.0008	A	403.43	0.0141	A’	403.44	0.0003
	A	290.01	0.0000	A”	290.08	0.0000	A	403.46	0.0003	A”	403.47	0.0151
	A	290.19	0.0003	A’	290.14	0.0002	A	404.03	0.0001	A”	403.86	0.0297
	A	290.26	0.0007	A’	290.25	0.0094	A	404.05	0.0121	A’	403.96	0.0002
	A	290.27	0.0096	A”	290.32	0.0005	A	404.10	0.0007	A’	404.00	0.0119
	A	290.44	0.0005	A’	290.39	0.0001	A	404.11	0.0002	A’	404.01	0.0001
	A	290.50	0.0020	A”	290.45	0.0026	A	404.12	0.0011	A’	404.06	0.0012
	A	290.54	0.0091	A’	290.51	0.0092	A	404.28	0.0216	A’	404.07	0.0007
	A	290.64	0.0007	A’	290.64	0.0007	A	404.39	0.0009	A”	404.23	0.0041
	A	290.70	0.0003	A’	290.66	0.0003	A	404.44	0.0012	A’	404.29	0.0213
	A	291.03	0.0004	A’	290.97	0.0004	A	404.51	0.0006	A’	404.34	0.0011
	A	291.23	0.0018	A’	291.23	0.0017	A	404.52	0.0005	A’	404.37	0.0009
				A’	291.34	0.0026				A”	404.45	0.0006
				A’	291.39	0.0005				A’	404.46	0.0005
				A’	291.44	0.0015				A”	404.53	0.0013
				A’	291.56	0.0004				A’	404.62	0.0002
				A”	291.60	0.0003				A”	404.75	0.0005
				A”	291.63	0.0001				A’	404.77	0.0007
				A’	291.65	0.0009				A”	404.95	0.0022
				A”	291.77	0.0021				A”	405.29	0.0012
				A”	291.81	0.0031				A”	405.58	0.0001
				A”	291.93	0.0010				A”	405.59	0.0082
IE	A	291.90		A	291.85		A	405.91		A’	405.84	

Table S12: Uracil. Oxygen CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at DFT Franck-Condon geometry (S_0, S_1 and S_2) and at the TD-DFT optimized S_1 geometry ($S_{1(min)}$) of Ref. **?**

	S_0			S_1			$S_{1(min)}$			S_2		
	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f
EE	A	533.24	0.03680	A	528.00	0.00987	A	528.51	0.01177	A	527.50	0.00000
	A	534.16	0.03423	A	528.92	0.00002	A	530.55	0.00001	A	528.42	0.00017
	A	536.44	0.00022	A	531.20	0.00000	A	532.42	0.00000	A	530.69	0.00003
	A	536.66	0.00044	A	531.42	0.00000	A	532.86	0.00000	A	530.92	0.00008
	A	537.26	0.00215	A	532.02	0.00000	A	532.96	0.00000	A	531.51	0.00001
	A	537.48	0.00109	A	532.24	0.00000	A	533.12	0.00021	A	531.74	0.00001
	A	537.55	0.00030	A	532.31	0.00043	A	533.23	0.00045	A	531.80	0.00241
	A	537.68	0.00028	A	532.44	0.00051	A	533.29	0.00000	A	531.94	0.00100
	A	537.71	0.00147	A	532.47	0.00000	A	533.53	0.00000	A	531.97	0.00004
	A	537.88	0.00177	A	532.64	0.00000	A	533.75	0.00000	A	532.14	0.00001
	A	537.94	0.00129	A	532.70	0.00000	A	533.79	0.00009	A	532.19	0.00000
	A	538.07	0.00226	A	532.83	0.00023	A	534.19	0.00000	A	532.32	0.00027
	A	538.20	0.00251	A	532.95	0.00000	A	534.27	0.00000	A	532.45	0.00000
	A	538.20	0.00175	A	532.96	0.00000	A	534.37	0.00000	A	532.45	0.00001
	A	538.52	0.00044	A	533.28	0.00000	A	534.37	0.00000	A	532.78	0.00000
	A	538.68	0.00038	A	533.44	0.00000	A	534.68	0.00000	A	532.93	0.00000
	A	538.81	0.00054	A	533.57	0.00000	A	535.00	0.00000	A	533.07	0.00000
	A	538.99	0.00074	A	533.75	0.00000	A	535.16	0.00000	A	533.24	0.00000
	A	539.34	0.00082	A	534.09	0.00003				A	533.59	0.00006
	A	539.65	0.00090	A	534.40	0.00000				A	533.90	0.00003
IE		539.67										

Table S13: Uracil. Oxygen CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at MP2/cc-pVTZ Franck-Condon geometry (S_0, S_1 and S_2) and at the EOM-CCSD/aug-cc-pVDZ optimized S_1 and S_2 geometry ($S_{1(min)}$ and $S_{2(min)}$) of Ref. **?** .

	S_0			S_1			$S_{1(min)}$			S_2			$S_{2(min)}$		
	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f
EE	A”	533.17	0.03670	A”	528.02	0.01001	A”	528.39	0.01139	A”	527.50	0.00049	A”	528.29	0.00057
	A”	534.13	0.03431	A”	528.98	0.00002	A”	530.16	0.00001	A”	528.46	0.00015	A”	529.38	0.00025
	A’	536.50	0.00018	A’	531.35	0.00000	A’	532.37	0.00000	A’	530.83	0.00003	A’	531.91	0.00003
	A’	536.68	0.00039	A’	531.53	0.00000	A’	532.62	0.00000	A’	531.01	0.00008	A’	531.95	0.00004
	A’	537.32	0.00222	A’	532.18	0.00000	A”	532.98	0.00028	A’	531.65	0.00001	A”	532.37	0.00153
	A’	537.49	0.00105	A’	532.34	0.00000	A’	533.01	0.00000	A’	531.82	0.00001	A”	532.53	0.00161
	A”	537.55	0.00026	A”	532.40	0.00042	A”	533.08	0.00052	A”	531.87	0.00234	A’	532.70	0.00001
	A”	537.66	0.00036	A”	532.51	0.00053	A’	533.26	0.00000	A”	531.98	0.00108	A’	532.71	0.00000
	A’	537.72	0.00159	A’	532.57	0.00000	A’	533.48	0.00000	A’	532.05	0.00005	A’	532.89	0.00007
	A”	537.96	0.00176	A”	532.81	0.00000	A’	533.60	0.00000	A”	532.29	0.00001	A”	533.35	0.00010
	A’	538.00	0.00148	A’	532.85	0.00000	A”	533.76	0.00009	A’	532.33	0.00000	A”	533.41	0.00000
	A”	538.08	0.00215	A”	532.93	0.00018	A’	534.11	0.00000	A”	532.41	0.00023	A’	533.41	0.00002
	A’	538.20	0.00200	A’	533.05	0.00000	A”	534.14	0.00000	A’	532.53	0.00001	A’	533.42	0.00000
	A’	538.26	0.00275	A’	533.11	0.00000	A’	534.15	0.00000	A’	532.59	0.00000	A’	533.69	0.00000
	A’	538.53	0.00042	A’	533.39	0.00000	A’	534.27	0.00000	A’	532.86	0.00000	A’	533.74	0.00000
	A’	538.75	0.00038	A’	533.60	0.00000	A’	534.42	0.00000	A’	533.07	0.00000	A”	534.56	0.00010
	A”	539.35	0.00078	A”	534.20	0.00003	A”	534.96	0.00003	A”	533.68	0.00006	A”	534.97	0.00005
	A”	539.72	0.00093	A”	534.57	0.00000	A”	535.30	0.00004	A”	534.04	0.00003	A”	535.15	0.00001
	A”	539.74	0.00083	A”	534.59	0.00005	A”	535.82	0.00000	A”	534.07	0.00006	A”	535.60	0.00000
IE		539.68													

Table S14: Uracil. Carbon CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at DFT Franck-Condon geometry (S_0, S_1 and S_2) and at the TD-DFT optimized S_1 geometry ($S_{1(min)}$) of Ref. **?**

	S_0			S_1			$S_{1(min)}$			S_2		
	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f
EE	A	285.84	0.03247	A	280.59	0.00095	A	282.01	0.00031	A	280.09	0.00000
	A	287.14	0.05869	A	281.89	0.00014	A	283.34	0.00006	A	281.39	0.00022
	A	288.35	0.00511	A	283.10	0.00000	A	284.44	0.00007	A	282.60	0.00001
	A	288.84	0.06900	A	283.59	0.00019	A	285.18	0.00000	A	283.09	0.00001
	A	289.34	0.01193	A	284.09	0.00049	A	285.65	0.00011	A	283.60	0.00068
	A	289.36	0.00412	A	284.11	0.00000	A	286.19	0.00000	A	283.61	0.00003
	A	289.59	0.00092	A	284.34	0.00000	A	286.48	0.00000	A	283.85	0.00002
	A	289.93	0.00285	A	284.68	0.00000	A	286.64	0.00000	A	284.18	0.00012
	A	289.96	0.01251	A	284.71	0.00000	A	286.82	0.00000	A	284.22	0.00006
	A	290.25	0.00413	A	285.00	0.00000	A	286.88	0.00000	A	284.50	0.00000
	A	290.25	0.08188	A	285.42	0.00000	A	287.07	0.00000	A	284.92	0.00002
	A	290.67	0.00137	A	285.85	0.00000	A	287.70	0.00000	A	285.36	0.00001
	A	291.10	0.00031	A	286.13	0.00000	A	288.03	0.00000	A	285.63	0.00004
	A	291.37	0.00172	A	286.15	0.00000	A	288.23	0.00000	A	285.66	0.00000
	A	291.40	0.00596	A	286.17	0.00000	A	288.25	0.00000	A	285.67	0.00001
	A	291.42	0.00081	A	286.25	0.00001	A	288.32	0.00000	A	285.76	0.00019
	A	291.50	0.00519	A	286.31	0.00000	A	288.42	0.00002	A	285.81	0.00001
	A	291.56	0.00265	A	286.63	0.00000	A	288.50	0.00000	A	286.13	0.00003
	A	291.88	0.00430	A	286.65	0.00000	A	288.51	0.00000	A	286.15	0.00000
	A	291.90	0.00105	A	286.93	0.00000	A	288.81	0.00000	A	286.44	0.00000
IE		291.94										

Table S15: Uracil. Carbon CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at MP2/cc-pVTZ Franck-Condon geometry (S_0, S_1 and S_2) and at the EOM-CCSD/aug-cc-pVDZ optimized S_1 and S_2 geometry ($S_{1(min)}$ and $S_{2(min)}$) of Ref. **?** .

	S_0			S_1			$S_{1(min)}$			S_2			$S_{2(min)}$		
	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f
EE	A”	285.84	0.03217	A”	280.17	0.00225	A”	281.84	0.00039	A”	280.17	0.00225	A”	281.02	0.00260
	A”	287.14	0.05880	A”	281.46	0.00018	A”	283.12	0.00007	A”	281.46	0.00018	A”	282.40	0.00008
	A’	288.39	0.00530	A’	282.72	0.00001	A”	284.35	0.00007	A’	282.72	0.00001	A’	284.03	0.00002
	A”	288.80	0.06906	A”	283.13	0.00001	A’	284.95	0.00000	A”	283.13	0.00001	A”	284.08	0.00000
	A”	289.29	0.01239	A”	283.61	0.00078	A”	285.44	0.00016	A”	283.61	0.00078	A”	284.62	0.00095
	A’	289.41	0.00419	A’	283.73	0.00003	A’	285.96	0.00000	A’	283.73	0.00003	A’	284.92	0.00004
	A’	289.65	0.00087	A’	283.97	0.00002	A’	286.26	0.00000	A’	283.97	0.00002	A’	285.23	0.00003
	A”	289.99	0.00294	A”	284.31	0.00011	A”	286.30	0.00000	A”	284.31	0.00011	A”	285.63	0.00018
	A’	290.01	0.01280	A’	284.33	0.00006	A’	286.59	0.00000	A’	284.33	0.00006	A’	285.86	0.00000
	A”	290.24	0.08196	A”	284.56	0.00000	A”	286.62	0.00000	A”	284.56	0.00000	A’	285.98	0.00004
	A’	290.30	0.00413	A’	284.63	0.00000	A’	286.81	0.00000	A’	284.63	0.00000	A’	286.27	0.00007
	A’	290.73	0.00137	A’	285.05	0.00002	A’	287.42	0.00000	A’	285.05	0.00002	A’	286.68	0.00005
	A’	291.15	0.00037	A’	285.48	0.00001	A’	287.77	0.00000	A’	285.48	0.00001	A’	286.90	0.00021
	A”	291.44	0.00194	A’	285.77	0.00000	A’	287.95	0.00000	A’	285.77	0.00000	A”	287.05	0.00005
	A’	291.45	0.00589	A”	285.77	0.00005	A’	287.99	0.00000	A”	285.77	0.00005	A”	287.12	0.00018
	A’	291.47	0.00096	A’	285.79	0.00001	A”	288.10	0.00000	A’	285.79	0.00001	A’	287.36	0.00001
	A”	291.56	0.00481	A”	285.88	0.00017	A’	288.22	0.00000	A”	285.88	0.00017	A”	287.46	0.00026
	A’	291.62	0.00249	A’	285.95	0.00001	A”	288.25	0.00001	A’	285.95	0.00001	A’	287.50	0.00003
	A”	291.95	0.00436	A”	286.27	0.00002	A”	288.25	0.00002	A”	286.27	0.00002	A”	287.94	0.00002
	A”	292.56	0.00817	A”	286.89	0.00010	A”	288.56	0.00000	A”	286.89	0.00010	A”	287.96	0.00040
IE		292.01													

Table S16: Uracil. Nitrogen CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at DFT Franck-Condon geometry (S_0, S_1 and S_2) and at the TD-DFT optimized S_1 geometry ($S_{1(min)}$) of Ref. **?**

	S_0			S_1			$S_{1(min)}$			S_2		
	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f	Symm.	ω_i	f
EE	A	403.61	0.01829	A	398.37	0.00129	A	399.26	0.00065	A	397.87	0.00000
	A	403.90	0.01320	A	398.65	0.00001	A	399.80	0.00001	A	398.15	0.00461
	A	403.99	0.01156	A	398.75	0.00000	A	400.68	0.00000	A	398.25	0.00000
	A	404.32	0.01174	A	399.07	0.00000	A	401.11	0.00000	A	398.58	0.00003
	A	404.69	0.00216	A	399.45	0.00024	A	401.24	0.00004	A	398.95	0.00061
	A	405.21	0.01256	A	399.96	0.00000	A	401.85	0.00000	A	399.46	0.00063
	A	405.37	0.00641	A	400.13	0.00000	A	401.97	0.00000	A	399.63	0.00001
	A	405.91	0.00526	A	400.66	0.00000	A	402.62	0.00000	A	400.17	0.00001
	A	406.00	0.00258	A	400.76	0.00000	A	402.64	0.00000	A	400.26	0.00000
	A	406.03	0.00007	A	400.79	0.00000	A	402.69	0.00000	A	400.29	0.00000
	A	406.14	0.00299	A	400.90	0.00001	A	402.82	0.00000	A	400.40	0.00000
	A	406.28	0.00202	A	401.04	0.00000	A	402.84	0.00000	A	400.54	0.00000
	A	406.39	0.00196	A	401.14	0.00000	A	403.12	0.00000	A	400.64	0.00010
	A	407.00	0.00224	A	401.76	0.00000	A	403.72	0.00000	A	401.26	0.00000
	A	407.02	0.00053	A	401.77	0.00000	A	403.73	0.00000	A	401.27	0.00000
	A	407.10	0.00049	A	401.86	0.00000	A	403.76	0.00000	A	401.36	0.00000
	A	407.13	0.00241	A	401.89	0.00000	A	403.99	0.00000	A	401.39	0.00001
	A	407.40	0.00093	A	402.15	0.00000	A	404.14	0.00000	A	401.66	0.00000
	A	407.55	0.00587									
	A	407.59	0.00028									
IE		408.00										

Table S17: Uracil. Nitrogen CVS-EOM-CCSD/6-311++G** K-edge excitation energies ω_i (EE, eV), oscillator strengths f, and ionization energies (IE, eV) at MP2/cc-pVTZ Franck-Condon geometry (S_0, S_1 and S_2) and at the EOM-CCSD/aug-cc-pVDZ optimized S_1 and S_2 geometry ($S_{1(min)}$ and $S_{2(min)}$) of Ref. **?** .

	S_0			S_1			$S_{1(min)}$			S_2			$S_{2(min)}$		
	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f	S.	ω_i	f
EE	A”	403.56	0.01854	A”	397.89	0.00000	A”	399.13	0.00079	A”	397.89	0.00001	A”	398.40	0.00411
	A”	403.86	0.01385	A”	398.19	0.00001	A”	399.56	0.00001	A”	398.19	0.00450	A”	398.64	0.00009
	A’	404.00	0.01196	A’	398.33	0.00000	A’	400.33	0.00000	A’	398.33	0.00000	A’	399.51	0.00000
	A’	404.33	0.01232	A’	398.66	0.00000	A’	400.74	0.00000	A’	398.66	0.00003	A’	399.85	0.00002
	A”	404.63	0.00225	A”	398.96	0.00000	A”	400.85	0.00007	A”	398.96	0.00062	A”	400.02	0.00050
	A”	405.15	0.01216	A”	399.48	0.00000	A”	401.42	0.00000	A”	399.48	0.00062	A”	400.76	0.00038
	A’	405.39	0.00665	A’	399.73	0.00000	A’	401.69	0.00000	A’	399.73	0.00001	A’	400.95	0.00001
	A’	405.95	0.00547	A’	400.28	0.00000	A’	402.31	0.00000	A’	400.28	0.00001	A’	401.48	0.00001
	A’	406.02	0.00271	A’	400.35	0.00000	A’	402.34	0.00000	A’	400.35	0.00000	A’	401.51	0.00000
	A’	406.06	0.00006	A’	400.39	0.00124	A’	402.35	0.00000	A’	400.39	0.00000	A’	401.57	0.00000
	A”	406.18	0.00304	A”	400.51	0.00001	A’	402.53	0.00000	A”	400.51	0.00000	A”	401.78	0.00001
	A’	406.30	0.00216	A’	400.63	0.00001	A”	402.56	0.00000	A’	400.63	0.00000	A’	401.83	0.00000
	A”	406.43	0.00197	A”	400.76	0.00000	A”	402.82	0.00000	A”	400.76	0.00010	A”	402.00	0.00007
	A’	407.03	0.00240	A’	401.37	0.00023	A’	403.36	0.00000	A’	401.37	0.00000	A’	402.44	0.00000
	A’	407.05	0.00052	A”	401.95	0.00000	A”	403.86	0.00000	A”	401.95	0.00000	A”	403.12	0.00000
	A’	407.12	0.00055	A”	402.13	0.00000	A”	404.00	0.00001	A”	402.13	0.00000	A”	403.29	0.00001
	A”	407.62	0.00017	A”	402.33	0.00000	A”	404.39	0.00000	A”	402.33	0.00000	A”	403.54	0.00000
	A”	407.80	0.00717	A”	402.58	0.00000	A”	404.57	0.00000	A”	402.58	0.00010	A”	403.79	0.00009
IE		408.04													

Table S18: fc-CVS-EOM-CCSD second moments of electron density using the 6-311++G** basis set with supplementary Rydberg functions

	Symm.	ω_i	f	$\langle x^2 \rangle$	$\langle y^2 \rangle$	$\langle z^2 \rangle$	$\langle r^2 \rangle$
Ne	B_{nu}	867.94	0.01063	50.0	18.3	18.3	86.7
	B_{nu}	869.55	0.00311	188.6	64.5	64.5	317.7
	B_{nu}	870.13	0.00133	421.7	142.2	142.2	706.2
H_2O	A_1	535.21	0.01288	12.7	8.5	11.7	32.9
	B_1	537.00	0.02604	19.1	8.4	10.9	38.3
	B_2	538.20	0.00670	20.1	47.4	20.3	87.8
	A_1	538.32	0.00399	25.2	23.4	42.4	90.9
	A_1	538.84	0.00247	33.7	40.2	55.0	128.9
NH_3	A_1	401.57	0.00635	15.5	13.7	15.5	44.7
	E	403.23	0.03859	28.2	13.7	14.9	56.8
	A_1	403.89	0.00556	20.7	38.1	20.7	79.5
	A_1	404.55	0.00155	47.3	60.1	47.8	155.3
	E	404.57	0.00800	46.4	20.4	31.0	97.8
	E	405.06	0.00572	118.6	54.9	53.3	226.8