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Supplementary - Gaunt and Breit Two-electron contributions to Mean-field Transformations and Fine Structure Splitting

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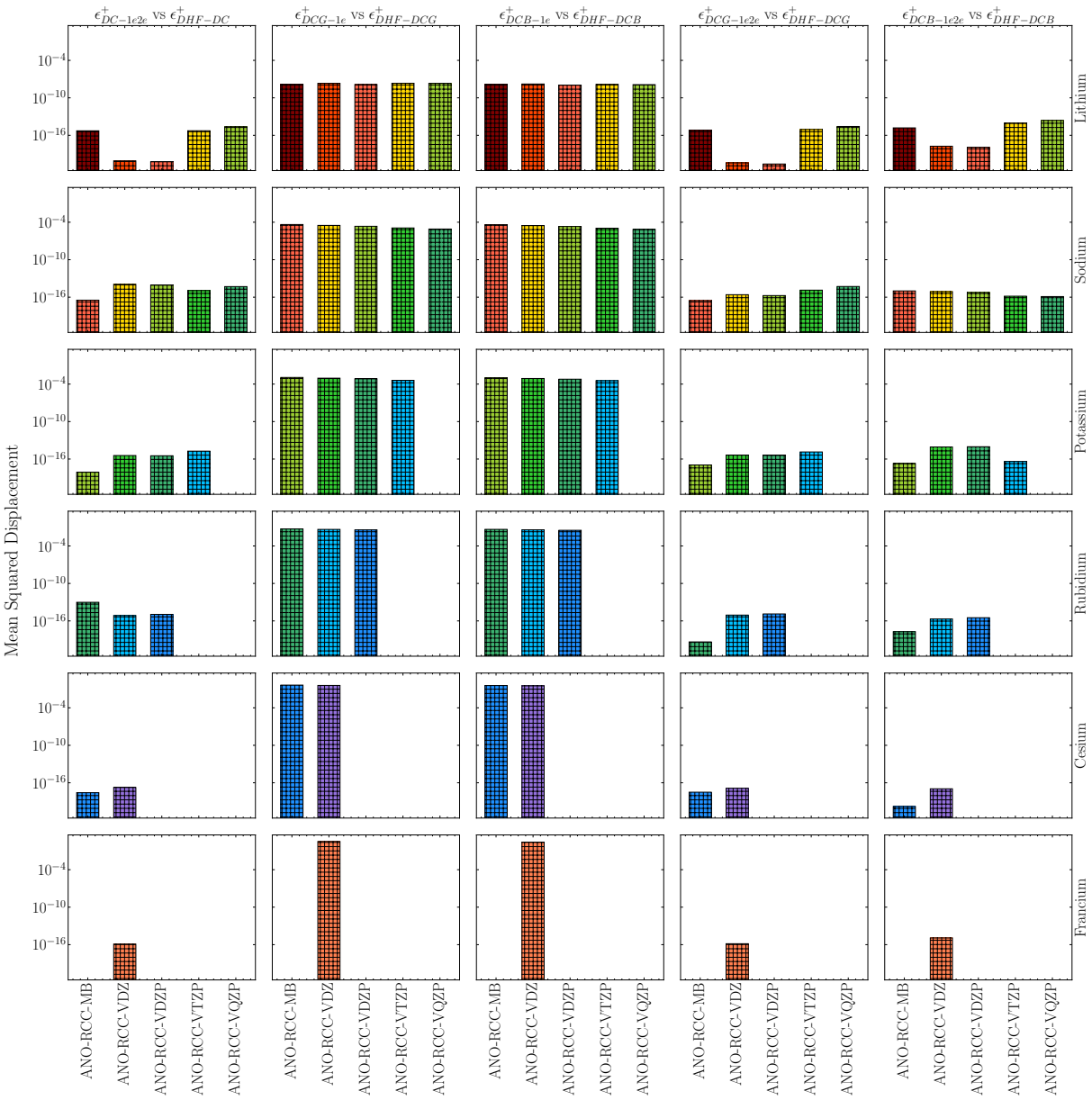

Figure S1: Mean squared displacement of positive energy spectrum after X2C$_{mmf}$ using DC-1e2e, DCG-1e, and DGB-1e, DCG-1e2e, and DCB-1e2e transformation versus the respective positive energy spectrum from 4c DHF using DC, DCG, and DCB Hamiltonian in a variety of basis sets ($MSD = \frac{1}{n}\sum_{i=1}^{n} |\epsilon^+_{i,4c-DHF} - \epsilon^+_{i,2c}|^2$, units are Hartree).

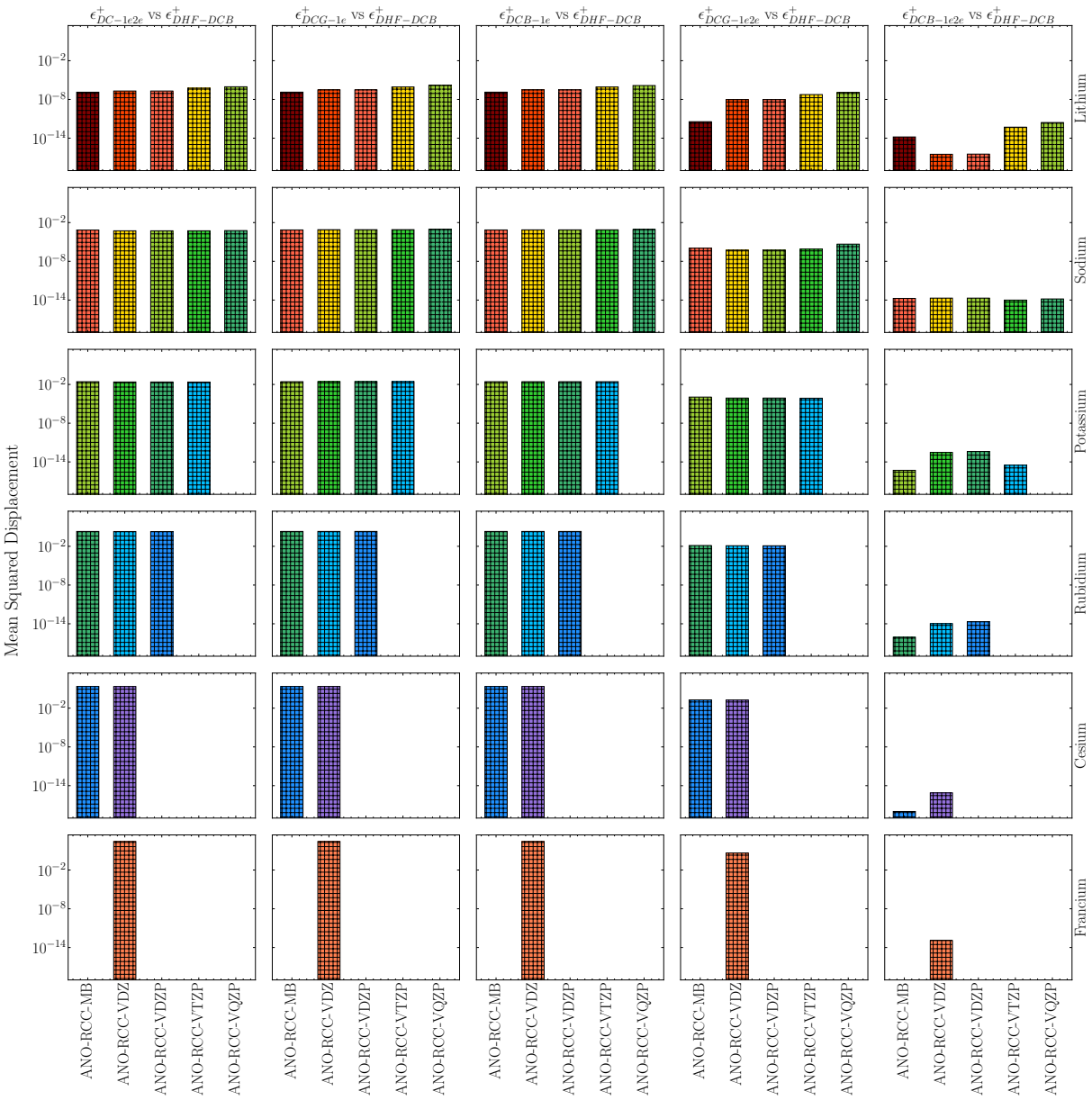

Figure S2: Mean squared displacement of positive energy spectrum after X2C$_{mmf}$ using DC-1e2e, DCG-1e, and DGB-1e, DCG-1e2e, and DCB-1e2e transformation versus the absolute value of positive energy spectrum from 4c DHF using the DCB Hamiltonian in a variety of basis sets ($MSD = \frac{1}{n}\sum_{i=1}^{n} |\epsilon^+_{i,4c-DHF-DCB} - \epsilon^+_{i,2c}|^2$, units are Hartree).

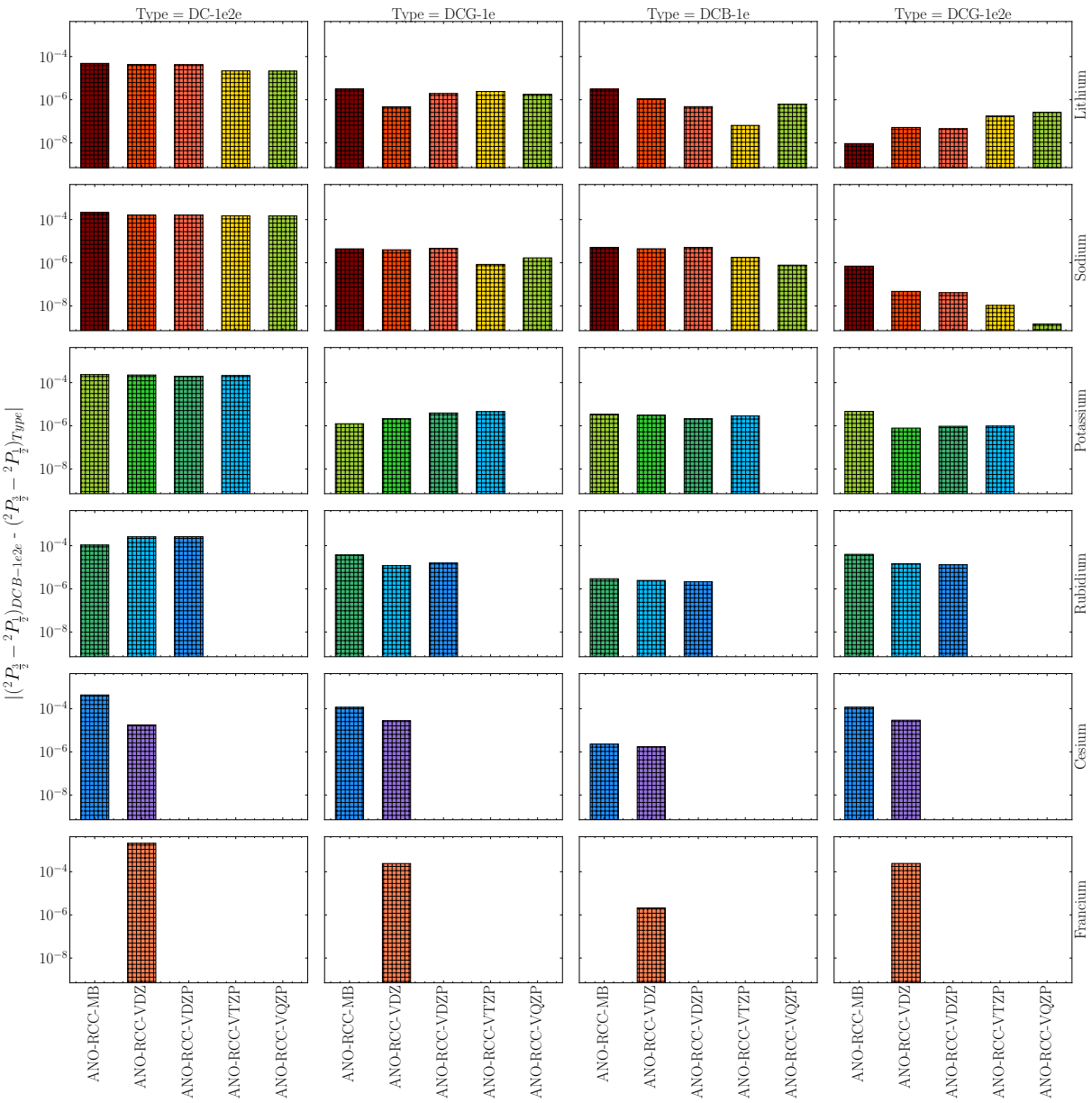

Figure S3: Absolute difference of fine structure splitting predicted using the DC-1e2e, DCG-1e, DCB-1e, and DCG-1e2e transformation versus the DCB-1e2e transformation for various basis sets calculated using EOM-CCSD-X2C$_{mmf}$-DHF in a variety of basis sets (units are eV).

Table S1: Lithium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-MB	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.8478	1.8467	1.8467	1.8467	1.8467	1.8467
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.8479	1.8468	1.8467	1.8467	1.8467	1.8467
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.8478	1.8437	1.8436	1.8436	1.8436	1.8436
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.8479	1.8438	1.8437	1.8437	1.8437	1.8437
ANO-RCC-VDZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.8478	1.8369	1.8368	1.8368	1.8368	1.8368
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.8479	1.8370	1.8369	1.8369	1.8369	1.8369
ANO-RCC-VTZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.8478	1.8434	1.8434	1.8434	1.8434	1.8434
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.8479	1.8436	1.8435	1.8435	1.8435	1.8435
ANO-RCC-VQZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.8478	1.8455	1.8454	1.8454	1.8454	1.8454
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.8479	1.8456	1.8455	1.8455	1.8456	1.8455

Table S2: Sodium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-MB	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	2.1023	2.0198	2.0199	2.0198	2.0199	2.0198
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	2.1044	2.0228	2.0227	2.0226	2.0227	2.0226
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	2.1023	1.9891	1.9891	1.9891	1.9891	1.9890
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	2.1044	1.9914	1.9913	1.9912	1.9913	1.9912
ANO-RCC-VDZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	2.1023	1.9870	1.9870	1.9870	1.9870	1.9870
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	2.1044	1.9894	1.9892	1.9892	1.9892	1.9892
ANO-RCC-VTZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	2.1023	2.0460	2.0459	2.0459	2.0459	2.0459
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	2.1044	2.0483	2.0481	2.0481	2.0481	2.0480
ANO-RCC-VQZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	2.1023	2.0755	2.0755	2.0755	2.0755	2.0754
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	2.1044	2.0778	2.0776	2.0776	2.0777	2.0776

Table S3: Potassium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-MB	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.6100	1.4465	1.4466	1.4466	1.4466	1.4466
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.6171	1.4539	1.4538	1.4537	1.4538	1.4537
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.6100	1.4467	1.4471	1.4470	1.4471	1.4469
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.6171	1.4533	1.4534	1.4533	1.4534	1.4533
ANO-RCC-VDZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.6100	1.5678	1.5681	1.5680	1.5681	1.5680
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.6171	1.5755	1.5756	1.5755	1.5756	1.5755
ANO-RCC-VTZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.6100	1.6275	1.6277	1.6276	1.6277	1.6276
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.6171	1.6352	1.6351	1.6350	1.6351	1.6350

Table S4: Rubidium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-MB	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.5596	1.3455	1.3449	1.3448	1.3448	1.3448
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.5890	1.3675	1.3668	1.3668	1.3668	1.3668
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.5596	1.3665	1.3676	1.3673	1.3676	1.3673
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.5890	1.3900	1.3908	1.3905	1.3908	1.3905
ANO-RCC-VDZP	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.5596	1.5174	1.5183	1.5180	1.5183	1.5180
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.5890	1.5414	1.5420	1.5417	1.5420	1.5417

Table S5: Cesium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-MB	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.3859	1.2419	1.2420	1.2419	1.2420	1.2419
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.4546	1.2927	1.2934	1.2932	1.2934	1.2932
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.3859	1.2962	1.2988	1.2982	1.2988	1.2982
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.4546	1.3492	1.3517	1.3511	1.3517	1.3511

Table S6: Francium's excitations for varying basis types and X2C$_{mmf}$ trasformation types, calculated using 4c DHF, Kramers unrestricted EOM-CCSD with eV units of energy.

Basis	Excitation	Experiment	DC-1e2e	DCG-1e	DCB-1e	DCG-1e2e	DCB-1e2e
ANO-RCC-VDZ	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	1.5172	1.8296	1.8407	1.8390	1.8407	1.8390
	$^2S_{\frac{1}{2}} \rightarrow {}^2P_{\frac{3}{2}}$	1.7264	1.9839	1.9973	1.9954	1.9973	1.9954

Table S7: Tabulated atom type, X2C$_{mmf}$ transformation type, basis, PySCF converged 4c DHF energy, converged unrestricted Kramers CCSD energy correction, and converged PySCF CCSD energy correction.

Atom	X2C$_{mmf}$ Type	Basis	$\mathbf{E}_{DHF}^{PySCF}$ [Ha]	$\Delta\ \mathbf{E}_{CCSD}^{This\ Work}$ [Ha]	$\Delta\ \mathbf{E}_{CCSD}^{PySCF}$ [Ha]
Li	DC-1e2e	ANO-RCC-MB	-7.43337869	-4.58212741E-05	-4.58212741E-05
Li	DC-1e2e	ANO-RCC-VDZ	-7.43349063	-1.61383218E-02	-1.61383218E-02
Li	DC-1e2e	ANO-RCC-VDZP	-7.43349063	-1.61401491E-02	-1.61401491E-02
Li	DC-1e2e	ANO-RCC-VTZP	-7.43350415	-3.65209750E-02	-3.65209750E-02
Li	DC-1e2e	ANO-RCC-VQZP	-7.43351115	-3.90337186E-02	-3.90337186E-02
Li	DCG-1e	ANO-RCC-MB	-7.43337869	-4.58212741E-05	-4.58212741E-05
Li	DCG-1e	ANO-RCC-VDZ	-7.43349063	-1.61383218E-02	-1.61383218E-02
Li	DCG-1e	ANO-RCC-VDZP	-7.43349063	-1.61401491E-02	-1.61401491E-02
Li	DCG-1e	ANO-RCC-VTZP	-7.43350415	-3.65209750E-02	-3.65209750E-02
Li	DCG-1e	ANO-RCC-VQZP	-7.43351115	-3.90337186E-02	-3.90337186E-02
Li	DCB-1e	ANO-RCC-MB	-7.43337869	-4.58212741E-05	-4.58212741E-05
Li	DCB-1e	ANO-RCC-VDZ	-7.43349063	-1.61383218E-02	-1.61383218E-02
Li	DCB-1e	ANO-RCC-VDZP	-7.43349063	-1.61401491E-02	-1.61401491E-02
Li	DCB-1e	ANO-RCC-VTZP	-7.43350415	-3.65209750E-02	-3.65209750E-02
Li	DCB-1e	ANO-RCC-VQZP	-7.43351115	-3.90337186E-02	-3.90337186E-02
Li	DCG-1e2e	ANO-RCC-MB	-7.43337869	-4.58212741E-05	-4.58212741E-05
Li	DCG-1e2e	ANO-RCC-VDZ	-7.43349063	-1.61383218E-02	-1.61383218E-02
Li	DCG-1e2e	ANO-RCC-VDZP	-7.43349063	-1.61401491E-02	-1.61401491E-02
Li	DCG-1e2e	ANO-RCC-VTZP	-7.43350415	-3.65209750E-02	-3.65209750E-02
Li	DCB-1e2e	ANO-RCC-MB	-7.43337869	-4.58212741E-05	-4.58212741E-05
Li	DCB-1e2e	ANO-RCC-VDZ	-7.43349063	-1.61383218E-02	-1.61383218E-02
Li	DCB-1e2e	ANO-RCC-VDZP	-7.43349063	-1.61401491E-02	-1.61401491E-02
Li	DCB-1e2e	ANO-RCC-VTZP	-7.43350415	-3.65209750E-02	-3.65209750E-02
Li	DCB-1e2e	ANO-RCC-VQZP	-7.43351115	-3.90337186E-02	-3.90337186E-02

Table S8: Tabulated atom type, X2C$_{mmf}$ transformation type, basis, PySCF converged 4c DHF energy, converged unrestricted Kramers CCSD energy correction, and converged PySCF CCSD energy correction.

Atom	X2C$_{mmf}$ Type	Basis	E_{DHF}^{PySCF} [Ha]	Δ $E_{CCSD}^{This\ Work}$ [Ha]	Δ E_{CCSD}^{PySCF} [Ha]
Na	DC-1e2e	ANO-RCC-MB	-162.05715650	-2.20078705E-04	-2.20078709E-04
Na	DC-1e2e	ANO-RCC-VDZ	-162.05720863	-1.17564643E-01	-1.17564643E-01
Na	DC-1e2e	ANO-RCC-VDZP	-162.05720863	-1.18638412E-01	-1.18638412E-01
Na	DC-1e2e	ANO-RCC-VTZP	-162.05723287	-2.03866922E-01	-2.03866922E-01
Na	DC-1e2e	ANO-RCC-VQZP	-162.05726902	-2.40431049E-01	-2.40431049E-01
Na	DCG-1e	ANO-RCC-MB	-162.05715650	-2.20078705E-04	-2.20078709E-04
Na	DCG-1e	ANO-RCC-VDZ	-162.05720863	-1.17564643E-01	-1.17564643E-01
Na	DCG-1e	ANO-RCC-VDZP	-162.05720863	-1.18638412E-01	-1.18638412E-01
Na	DCG-1e	ANO-RCC-VTZP	-162.05723287	-2.03866922E-01	-2.03866922E-01
Na	DCG-1e	ANO-RCC-VQZP	-162.05726902	-2.40431049E-01	-2.40431049E-01
Na	DCB-1e	ANO-RCC-MB	-162.05715650	-2.20078705E-04	-2.20078709E-04
Na	DCB-1e	ANO-RCC-VDZ	-162.05720863	-1.17564643E-01	-1.17564643E-01
Na	DCB-1e	ANO-RCC-VDZP	-162.05720863	-1.18638412E-01	-1.18638412E-01
Na	DCB-1e	ANO-RCC-VTZP	-162.05723287	-2.03866922E-01	-2.03866922E-01
Na	DCB-1e	ANO-RCC-VQZP	-162.05726902	-2.40431049E-01	-2.40431049E-01
Na	DCG-1e2e	ANO-RCC-MB	-162.05715650	-2.20078705E-04	-2.20078709E-04
Na	DCG-1e2e	ANO-RCC-VDZ	-162.05720863	-1.17564643E-01	-1.17564643E-01
Na	DCG-1e2e	ANO-RCC-VDZP	-162.05720863	-1.18638412E-01	-1.18638412E-01
Na	DCG-1e2e	ANO-RCC-VTZP	-162.05723287	-2.03866922E-01	-2.03866922E-01
Na	DCG-1e2e	ANO-RCC-VQZP	-162.05726902	-2.40431049E-01	-2.40431049E-01
Na	DCB-1e2e	ANO-RCC-MB	-162.05715650	-2.20078705E-04	-2.20078709E-04
Na	DCB-1e2e	ANO-RCC-VDZ	-162.05720863	-1.17564643E-01	-1.17564643E-01
Na	DCB-1e2e	ANO-RCC-VDZP	-162.05720863	-1.18638412E-01	-1.18638412E-01
Na	DCB-1e2e	ANO-RCC-VTZP	-162.05723287	-2.03866922E-01	-2.03866922E-01
Na	DCB-1e2e	ANO-RCC-VQZP	-162.05726902	-2.40431049E-01	-2.40431049E-01

Table S9: Tabulated atom type, X2C$_{mmf}$ transformation type, basis, PySCF converged 4c DHF energy, converged unrestricted Kramers CCSD energy correction, and converged PySCF CCSD energy correction.

Atom	X2C$_{mmf}$ Type	Basis	E_{DHF}^{PySCF} [Ha]	Δ $E_{CCSD}^{This\ Work}$ [Ha]	Δ E_{CCSD}^{PySCF} [Ha]
K	DC-1e2e	ANO-RCC-MB	-601.33547064	-2.81712233E-04	-2.81712226E-04
K	DC-1e2e	ANO-RCC-VDZ	-601.33574000	-4.19427003E-02	-4.19427003E-02
K	DC-1e2e	ANO-RCC-VDZP	-601.33574000	-1.88640717E-01	-1.88640717E-01
K	DC-1e2e	ANO-RCC-VTZP	-601.33586043	-2.60677803E-01	-2.60677804E-01
K	DCG-1e	ANO-RCC-MB	-601.33547064	-2.81712233E-04	-2.81712226E-04
K	DCG-1e	ANO-RCC-VDZ	-601.33574000	-4.19427003E-02	-4.19427003E-02
K	DCG-1e	ANO-RCC-VDZP	-601.33574000	-1.88640717E-01	-1.88640717E-01
K	DCG-1e	ANO-RCC-VTZP	-601.33586043	-2.60677803E-01	-2.60677804E-01
K	DCB-1e	ANO-RCC-MB	-601.33547064	-2.81712233E-04	-2.81712226E-04
K	DCB-1e	ANO-RCC-VDZ	-601.33574000	-4.19427003E-02	-4.19427003E-02
K	DCB-1e	ANO-RCC-VDZP	-601.33574000	-1.88640717E-01	-1.88640717E-01
K	DCB-1e	ANO-RCC-VTZP	-601.33586043	-2.60677803E-01	-2.60677804E-01
K	DCG-1e2e	ANO-RCC-MB	-601.33547064	-2.81712233E-04	-2.81712226E-04
K	DCG-1e2e	ANO-RCC-VDZ	-601.33574000	-4.19427003E-02	-4.19427003E-02
K	DCG-1e2e	ANO-RCC-VDZP	-601.33574000	-1.88640717E-01	-1.88640717E-01
K	DCG-1e2e	ANO-RCC-VTZP	-601.33586043	-2.60677803E-01	-2.60677804E-01
K	DCB-1e2e	ANO-RCC-MB	-601.33547064	-2.81712233E-04	-2.81712226E-04
K	DCB-1e2e	ANO-RCC-VDZ	-601.33574000	-4.19427003E-02	-4.19427003E-02
K	DCB-1e2e	ANO-RCC-VDZP	-601.33574000	-1.88640717E-01	-1.88640717E-01
K	DCB-1e2e	ANO-RCC-VTZP	-601.33586043	-2.60677803E-01	-2.60677804E-01

Table S10: Tabulated atom type, X2C$_{mmf}$ transformation type, basis, PySCF converged 4c DHF energy, converged unrestricted Kramers CCSD energy correction, and converged PySCF CCSD energy correction.

Atom	X2C$_{mmf}$ Type	Basis	E_{DHF}^{PySCF} [Ha]	Δ $E_{CCSD}^{This\ Work}$ [Ha]	Δ E_{CCSD}^{PySCF} [Ha]
Rb	DC-1e2e	ANO-RCC-MB	-2989.57808707	-2.54348217E-04	-2.54348209E-04
Rb	DC-1e2e	ANO-RCC-VDZ	-2989.58340243	-2.93237276E-02	-2.93237276E-02
Rb	DC-1e2e	ANO-RCC-VDZP	-2989.58353577	-1.65029862E-01	-1.65029862E-01
Rb	DCG-1e	ANO-RCC-MB	-2989.57808707	-2.54348217E-04	-2.54348209E-04
Rb	DCG-1e	ANO-RCC-VDZ	-2989.58340243	-2.93237276E-02	-2.93237276E-02
Rb	DCG-1e	ANO-RCC-VDZP	-2989.58353577	-1.65029862E-01	-1.65029862E-01
Rb	DCB-1e	ANO-RCC-MB	-2989.57808707	-2.54348217E-04	-2.54348209E-04
Rb	DCB-1e	ANO-RCC-VDZ	-2989.58340243	-2.93237276E-02	-2.93237276E-02
Rb	DCB-1e	ANO-RCC-VDZP	-2989.58353577	-1.65029862E-01	-1.65029862E-01
Rb	DCG-1e2e	ANO-RCC-MB	-2989.57808707	-2.54348217E-04	-2.54348209E-04
Rb	DCG-1e2e	ANO-RCC-VDZ	-2989.58340243	-2.93237276E-02	-2.93237276E-02
Rb	DCG-1e2e	ANO-RCC-VDZP	-2989.58353577	-1.65029862E-01	-1.65029862E-01
Rb	DCB-1e2e	ANO-RCC-MB	-2989.57808707	-2.54348217E-04	-2.54348209E-04
Rb	DCB-1e2e	ANO-RCC-VDZ	-2989.58340243	-2.93237276E-02	-2.93237276E-02
Rb	DCB-1e2e	ANO-RCC-VDZP	-2989.58353577	-1.65029862E-01	-1.65029862E-01
Cs	DC-1e2e	ANO-RCC-MB	-8051.50915614	-2.97025801E-04	-2.97025799E-04
Cs	DC-1e2e	ANO-RCC-VDZ	-8051.57094011	-2.52678284E-02	-2.52678285E-02
Cs	DCG-1e	ANO-RCC-MB	-8051.50915614	-2.97025801E-04	-2.97025799E-04
Cs	DCG-1e	ANO-RCC-VDZ	-8051.57094011	-2.52678284E-02	-2.52678285E-02
Cs	DCB-1e	ANO-RCC-MB	-8051.50915614	-2.97025801E-04	-2.97025799E-04
Cs	DCB-1e	ANO-RCC-VDZ	-8051.57094011	-2.52678284E-02	-2.52678285E-02
Cs	DCG-1e2e	ANO-RCC-MB	-8051.50915614	-2.97025801E-04	-2.97025799E-04
Cs	DCG-1e2e	ANO-RCC-VDZ	-8051.57094011	-2.52678284E-02	-2.52678285E-02
Cs	DCB-1e2e	ANO-RCC-MB	-8051.50915614	-2.97025801E-04	-2.97025799E-04
Cs	DCB-1e2e	ANO-RCC-VDZ	-8051.57094011	-2.52678284E-02	-2.52678285E-02
Fr	DC-1e2e	ANO-RCC-VDZ	-28955.29686485	-2.81453993E-02	-
Fr	DCG-1e	ANO-RCC-VDZ	-28955.29686485	-2.81453993E-02	-
Fr	DCB-1e	ANO-RCC-VDZ	-28955.29686485	-2.81453993E-02	-
Fr	DCG-1e2e	ANO-RCC-VDZ	-28955.29686485	-2.81453993E-02	-
Fr	DCB-1e2e	ANO-RCC-VDZ	-28955.29686485	-2.81453993E-02	-

Table S11: Time required to perform a variety of X2C$_{mmf}$ transformation for a variety of basis for a Sodium atom.

Atom	Basis	X2C$_{mmf}$ Type	Transformation Time [sec]
Na	ANO-RCC-VDZ	DC-1e2e	1.2531
Na	ANO-RCC-VDZ	DCG-1e	1.2207
Na	ANO-RCC-VDZ	DCB-1e	1.2106
Na	ANO-RCC-VDZ	DCB-1e2e	1.9817
Na	ANO-RCC-VDZ	DCB-1e2e	10.2324
Na	ANO-RCC-VDZP	DC-1e2e	2.6609
Na	ANO-RCC-VDZP	DCG-1e	2.76
Na	ANO-RCC-VDZP	DCB-1e	2.8776
Na	ANO-RCC-VDZP	DCG-1e2e	4.4292
Na	ANO-RCC-VDZP	DCB-1e2e	23.662
Na	ANO-RCC-VTZP	DC-1e2e	11.5411
Na	ANO-RCC-VTZP	DCG-1e	11.555
Na	ANO-RCC-VTZP	DCB-1e	11.5175
Na	ANO-RCC-VTZP	DCG-1e2e	20.0802
Na	ANO-RCC-VTZP	DCB-1e2e	64.6176
Na	ANO-RCC-VQZP	DC-1e2e	55.9794
Na	ANO-RCC-VQZP	DCG-1e	56.7785
Na	ANO-RCC-VQZP	DCB-1e	56.455
Na	ANO-RCC-VQZP	DCG-1e2e	113.3471
Na	ANO-RCC-VQZP	DCB-1e2e	180.4449