Supporting Information:

On the Performance of Delta-Coupled-Cluster Methods for Calculations of Core-Ionization Energies of First-Row Elements

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Table S1: The structure of ethyl trifluoroacetate ($CF_3COOCH_2CH_3$) in the C_s conformer obtained from a CCSD(T)/ANO1 calculation (Cartesian coordinates in Bohr).

atom	x	y	z
O	2.10457	0.46241	0.00000
C	0.17019	-1.13895	0.00000
O	0.26301	-3.40850	0.00000
C	-2.33157	0.36076	0.00000
F	-4.28996	-1.19974	0.00000
F	-2.47994	1.83390	-2.04537
F	-2.47994	1.83390	2.04537
C	4.57811	-0.72714	0.00000
H	4.71685	-1.92617	-1.67076
H	4.71685	-1.92617	1.67076
C	6.51383	1.37227	0.00000
H	6.30766	2.55507	-1.67454
H	6.30766	2.55507	1.67454
H	8.40889	0.55808	0.00000

Table S2: The structure of ethyl trifluoroacetate ($CF_3COOCH_2CH_3$) in the C_1 conformer obtained from a CCSD(T)/ANO1 calculation (Cartesian coordinates in Bohr).

atom	x	y	z
O	1.92362	1.20559	0.67819
C	0.41542	-0.77494	0.34769
O	0.98600	-2.97385	0.38360
C	-2.31081	0.15681	-0.11166
F	-3.86399	-1.78579	-0.40407
F	-3.11871	1.54299	1.83673
F	-2.41216	1.58437	-2.19259
C	4.57287	0.60795	1.09064
H	5.31033	2.26937	2.05107
H	4.68528	-1.02586	2.33893
C	5.90381	0.13472	-1.40063
H	5.13458	-1.53275	-2.33392
H	5.70474	1.76356	-2.64778
H	7.91301	-0.18323	-1.05370