Supporting Information for "Reference Energies for Non-Relativistic Core Ionization Potentials"

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TABLE S1. Core IPs (in eV) in the ACVTZ basis set calculated using CVS-IP-EOM-CC2, -CCSD, -CC3, -CCSDT, -CC4, -CCSDTQ, ΔROHF, ΔUHF, ΔUMP2, and G_0W_0@PBEh(α). The results for CVS-IP-EOM-CC4 and -CCSDTQ have been obtained using a composite basis set scheme using CVS-IP-EOM-CCSDT and the ACVDZ basis set [see Eq. (1) of the main manuscript]. The results for G_0W_0@PBEh(α) have been obtained using $\alpha = 0.45$ and $\alpha = 0.70$ for second- and third-row atoms, respectively.

IP	CC2	CCSD	CC3	CCSDT	CC4	CCSDTQ	ΔROHF	ΔUHF	ΔUMP2	G_0W_0@PBEh(α)
H**F***	691.15	695.81	692.74	693.80	694.12	694.09	693.22	692.94	694.34	692.44 (0.67)
H_2**O***	537.98	541.48	538.87	539.61	539.87	539.86	539.29	539.01	540.06	538.99 (0.66)
N$^*H_3$	405.10	407.04	405.17	405.47	405.63	405.64	405.40	405.12	405.78	405.30 (0.66)
C$^*H_4$	291.64	291.99	290.80	290.78	290.86	290.88	290.85	290.61	290.98	290.96 (0.71)
B**F***	692.80	697.78	694.02	695.35	695.40	695.41	694.60	694.32	695.86	694.01 (0.62)
C**O***	540.29	544.26	541.54	542.24	542.53	542.43	541.61	541.30	542.92	541.76 (0.66)
C*O	297.73	297.66	296.57	296.47	296.31	296.31	297.20	296.40	297.75	296.14 (0.70)
$\mathbf{N}_2^*$	409.54	411.28	410.05	410.00	409.90	409.95	410.15	409.42	411.09	409.75 (0.69)
$\mathbf{F}_2^*$	694.31	698.58	695.57	696.26	696.46	696.44	694.98	694.55	697.13	695.62 (0.67)
HC**N***	406.06	408.33	406.55	406.73	406.74	406.78	406.66	406.07	407.53	406.66 (0.65)
H**C***N	294.22	294.63	293.68	293.55	293.42	293.43	293.75	292.88	294.99	293.54 (0.70)
HN**O***	39.980	543.56	540.89	541.47	541.60	541.60	540.64	540.29	542.10	541.03 (0.63)
H**N***O	410.17	411.57	409.96	409.98	409.89	409.91	410.01	408.77	411.29	410.02 (0.65)
HO**F***	691.71	696.48	692.96	693.92	694.16	694.13	692.53	692.20	694.68	693.26 (0.66)
H**O***F	541.64	544.49	542.07	542.46	542.56	542.57	542.15	541.32	543.74	542.41 (0.67)
NH_2**F***	690.41	695.28	691.58	692.69	692.95	692.91	691.57	691.26	693.36	691.94 (0.65)
N$^*H_2$F	408.74	410.13	408.34	408.43	408.48	408.49	408.56	408.03	409.29	408.62 (0.68)
CH_3**F***	689.92	694.73	691.11	692.29	692.56	692.53	691.45	691.17	692.86	691.32 (0.66)
C$^*H_3$F	294.82	294.89	293.67	293.58	293.60	293.61	293.77	239.50	293.84	293.84 (0.72)
CH_2**O***	537.50	541.43	538.28	539.15	539.35	539.34	538.30	537.99	539.65	538.74 (0.63)
C$^*H_2$O	295.95	295.94	294.73	294.60	294.52	294.52	294.87	293.87	295.68	294.84 (0.71)
CH_2**N***H	405.16	407.28	405.18	405.46	405.57	405.58	405.04	404.71	405.83	405.52 (0.64)
C$^*H_2$NH	293.77	294.01	292.75	292.65	292.62	292.62	292.68	292.02	293.45	292.90 (0.69)
$\mathbf{C}_2^*H_2$	291.95	292.69	291.46	291.40	291.34	291.36	291.41	290.72	292.29	291.49 (0.66)
Si**O***	534.55	539.87	534.86	537.10	536.86	537.08	535.99	535.68	537.52	536.46 (0.56)
P**N***	404.46	407.75	405.10	405.71	405.71	405.71	405.52	404.61	406.90	405.88 (0.59)
C*S	294.75	295.26	294.02	293.75	293.53	293.51	294.71	294.63	293.74	294.11 (0.53)
$\mathbf{C}_2^*H_4$	291.80	292.27	290.89	290.83	290.86	290.88	290.66	290.27	291.23	291.06 (0.66)
CH_3**O***H	537.30	540.87	537.99	538.75	539.01	538.99	538.28	537.99	539.26	538.48 (0.66)
C$^*H_3$OH	293.55	293.76	292.53	292.45	292.52	292.52	292.56	292.29	292.74	292.74 (0.72)
C$\mathbf{O}_2^*$	539.38	543.46	540.20	541.14	541.22	541.19	540.82	540.53	541.47	540.85 (0.65)
C$^*O_2$	299.46	299.57	298.13	298.06	297.84	297.83	299.44	299.15	297.56	298.21 (0.74)
NN**O***	539.16	543.69	540.06	541.37	541.46	541.38	540.66	540.31	542.56	540.85 (0.63)
N**N***O	412.78	414.79	412.84	413.03	412.70	412.75	413.95	413.27	414.37	413.18 (0.70)
N*NO	408.27	410.72	408.79	408.85	408.72	408.78	409.41	408.54	410.06	408.99 (0.66)
HNC**O***	538.46	542.63	539.06	540.11	540.12	540.10	539.65	539.35	540.50	539.77 (0.63)
H**N***CO	405.74	408.18	405.96	406.33	406.41	406.40	406.23	405.95	406.58	406.43 (0.67)
HN**C***O	297.70	297.92	296.41	296.31	296.10	296.08	297.45	296.63	298.23	296.50 (0.71)

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TABLE S2. Core IPs (in eV) in the ACVTZ basis set calculated using CVS-IP-EOM-CC2, -CCSD, -CC3, -CCSDT, -CC4, -CCSDTQ, ΔROHF, ΔUHF, ΔUMP2, and G_0W_0@PBEh(α). The results for CVS-IP-EOM-CC4 and -CCSDTQ have been obtained using a composite basis set scheme using CVS-IP-EOM-CCSDT and the ACVDZ basis set [see Eq. (1) of the main manuscript]. The results for G_0W_0@PBEh(α) have been obtained using $\alpha = 0.45$ and $\alpha = 0.70$ for second- and third-row atoms, respectively.

IP	CC2	CCSD	CC3	CCSDT	CC4	CCSDTQ	ΔROHF	ΔUHF	ΔUMP2	G_0W_0@PBEh(α)
F*CHO	691.51	696.44	692.54	693.82	693.86		693.26	692.96	694.40	692.84 (0.64)
FCH**O***	538.33	542.20	539.11	539.93	540.07		539.28	538.99	540.39	539.52 (0.64)
F**C***HO	298.77	298.72	297.42	297.30	297.16		297.89	296.97	298.52	297.52 (0.66)
HCO**O***H	539.07	542.70	539.71	540.49	540.62		540.21	539.91	540.95	540.20 (0.65)
HC**O***OH	537.12	541.13	537.79	538.72	538.81		538.04	537.75	539.15	538.27 (0.62)
H**C***OOH	297.41	297.46	296.12	296.00	295.89		296.60	296.47	296.49	296.21 (0.72)
H_2C**N***N	409.67	411.75	409.52	409.72	409.58		409.47	409.21	410.40	409.87 (0.60)
H_2CN**N***	407.31	409.52	407.16	407.35	407.21		407.16	406.45	408.51	407.27 (0.59)
H_2**C***NN	292.29	293.26	291.76	291.75	291.71		291.59	291.30	292.18	291.91 (0.66)
H_2CC**O***	538.60	542.73	539.02	540.11	540.10		539.29	538.99	540.66	539.66 (0.60)
H_2C**C***O	296.63	296.75	295.21	295.06	294.87		295.49	294.35	296.18	295.30 (0.62)
H_2**C***CO	291.85	292.59	291.12	291.14	291.13		291.16	290.91	291.23	291.40 (0.68)
C$^*H_2S$	293.48	294.07	292.56	292.44	292.38		292.58	291.70	293.22	292.92 (0.62)
O*CS	538.83	543.22	539.10	540.36	540.19		539.85	539.45	541.17	539.99 (0.59)
O**C***S	297.11	297.68	295.99	295.83	295.60		297.19	296.86	295.39	296.21 (0.66)
CH_3C**N***	405.13	407.39	405.36	405.56	405.56		405.39	404.91	406.14	405.54 (0.64)
CH_3**C***N	293.46	294.03	292.99	292.87	292.77		293.06	292.65	293.10	293.04 (0.72)
C$^*H_3CN$	293.74	294.16	292.87	292.86	292.88		292.91	292.21	294.26	292.95 (0.71)
CH_3**N***C	405.74	408.26	406.28	406.52	406.73		406.12	405.79	407.13	406.65 (0.67)
C$^*H_3NC$	294.33	294.71	293.42	293.35	293.44		293.42	292.10	293.88	293.59 (0.72)
CH_3N**C***	293.88	294.07	292.67	292.57	292.40		293.03	293.17	293.68	292.53 (0.66)
NH_2CH**O***	535.91	540.02	536.43	537.48	537.48		536.72	536.43	537.87	536.96 (0.60)
N$^*H_2CHO$	406.11	408.23	406.10	406.43	406.50		406.31	406.04	406.77	406.48 (0.65)
NH_2**C***HO	296.05	296.20	294.80	294.69	294.58		295.30	295.07	294.75	294.85 (0.70)
CH_3N**O***	539.09	542.76	539.66	540.34	540.37		539.40	539.08	540.90	539.85 (0.60)
CH_3**N***O	409.48	411.02	409.18	409.23	409.14		409.26	407.86	410.60	409.37 (0.62)
C$^*H_3NO$	293.17	293.48	292.10	292.05	292.04		292.30	292.03	292.20	292.45 (0.70)
CH_2CH**F***	690.67	695.51	691.57	692.89	692.99		692.00	691.71	693.43	691.72 (0.62)
CH_2**C***HF	294.72	295.01	293.61	293.50	293.47		293.43	292.98	294.02	293.73 (0.45)
C$^*H_2CHF$	291.97	292.46	291.06	291.03	291.03		290.92	290.60	291.30	291.26 (0.45)
CH_3CH**O***	536.87	540.83	537.45	538.38	538.49		537.48	537.19	538.84	537.92 (0.61)
CH_3**C***HO	295.42	295.57	294.27	294.14	294.08		294.41	293.44	295.38	294.41 (0.70)
C$^*H_3CHO$	292.39	292.76	291.44	291.42	291.46		291.57	291.31	291.81	291.76 (0.71)
N$^*{}_2CH_2$	408.01	409.93	408.02	408.13	408.10		407.81	407.19	409.12	408.37 (0.65)
N_2**C**$^*H_2$	293.91	294.32	293.06	292.98	292.96		293.05	292.74	293.26	293.36 (0.65)
H**Cl***	2821.32	2824.61	2820.71	2821.45	2821.37	2821.43	2821.67	2821.38	2821.21	2821.42 (0.78)
H_2**S***	2471.87	2474.94	2471.06	2471.76	2471.66	2471.72	2472.06	2471.78	2472.01	2472.05 (0.79)
P$^*H_3$	2146.06	2148.92	2145.22	2145.83	2145.71	2145.77	2146.28	2146.00	2146.05	2146.36 (0.80)
Si$^*H_4$	1843.46	1846.26	1842.87	1843.40	1843.29	1843.33	1843.84	1843.56	1844.00	1843.96 (0.81)
C**S***	2472.82	2476.14	2472.14	2472.87	2472.80	2472.82	2472.86	2472.57	2473.36	2473.12 (0.78)
P*N	2147.57	2150.62	2147.19	2147.75	2147.50	2147.58	2148.31	2148.05	2147.18	2147.63 (0.69)
Si*O	1845.20	1848.18	1845.09	1845.63	1845.31	1845.39	1846.38	1846.12	1845.81	1845.73 (0.80)
P$^*{}_2$	2146.10	2149.47	2145.03	2145.91	2145.62	2145.71	2146.19	2145.94	2148.76	2146.55 (0.62)
Cl$^*{}_2$	2822.29	2825.69	2821.25	2822.09	2821.86	2821.93	2822.10	2821.81	2822.49	2822.45 (0.77)
CH_2**S***	2471.39	2474.68	2470.41	2471.23	2471.05	2471.13	2471.03	2470.74	2471.51	2471.60 (0.77)
OC**S***	2472.28	2475.61	2471.43	2472.25	2471.99	2472.07	2472.44	2472.16	2472.40	2472.70 (0.78)