

Supporting Information for

Partitioned EOMEA-MBPT(2): An Efficient N^5 Scaling Method for Calculation of Electron Affinities

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URACIL

Cartesian Coordinate

N	-1.199367	0.960746	0.069619
C	-0.034239	1.764602	-0.104318
H	-0.157030	2.790587	0.214353
C	1.211023	1.100068	-0.002163
H	2.126625	1.670370	0.022013
C	1.310963	-0.293494	0.002391
O	2.323801	-1.034380	0.035467
N	0.035200	-0.972450	-0.059347
H	0.070795	-1.976596	-0.028753
C	-1.207939	-0.401417	0.007847
O	-2.256589	-1.064639	0.007599
H	-2.107759	1.371159	-0.046589

aug-cc-pVDZ basis

THE NUCLEAR REPULSION ENERGY = 353.72900716 a.u.

FINAL SCF ENERGY IS = -412.49853479 a.u.

SECOND ORDER CORRELATION ENERGY = -1.33572998 a.u.

FINAL TARGET STATE ENERGY = -413.84066699 a.u.

aug-cc-pVTZ basis

THE NUCLEAR REPULSION ENERGY = 353.72900716 a.u.

FINAL SCF ENERGY IS = -412.56615767 a.u.

SECOND ORDER CORRELATION ENERGY = -1.50784100 a.u.

FINAL TARGET STATE ENERGY = -414.06899008 a.u.

Adenine

Cartesian Coordinate

C	1.22540300	-0.60749800	-0.00107700
C	-0.17733600	-0.51701700	-0.00098700
C	-0.70815400	0.77115800	-0.00074700
N	-0.02173100	1.91421300	-0.00023000
C	1.29113700	1.69606300	0.00101900
N	1.93953000	0.52527900	0.00116000
N	-1.17903800	-1.46962000	0.00029600
C	-2.28382500	-0.77470200	0.00092400
N	-2.06968800	0.58479000	0.00007400
N	1.87420000	-1.79142900	-0.01041000
H	-3.27898300	-1.18865300	0.00197300
H	1.35925200	-2.65117200	0.03220700
H	2.87685700	-1.79952000	0.03198500
H	1.92137100	2.57734700	0.00239000
H	-2.76475900	1.31134100	0.00041900

aug-cc-pVDZ basis

THE NUCLEAR REPULSION ENERGY = 503.68689701 a.u.

FINAL SCF ENERGY IS = -464.58967519 a.u.

SECOND ORDER CORRELATION ENERGY = -1.59930395 a.u.

FINAL TARGET STATE ENERGY = -466.17211140 a.u.

aug-cc-pVTZ basis

THE NUCLEAR REPULSION ENERGY = 503.68689700 a.u.

FINAL SCF ENERGY IS = -464.65868639 a.u.

SECOND ORDER CORRELATION ENERGY = -1.80123237 a.u.

FINAL TARGET STATE ENERGY = -466.44480870 a.u.

Guanine

Cartesian Coordinate

N	-1.66950500	-1.66317400	-0.00412800
C	-0.51642600	-0.92457400	-0.00030000
C	-0.81813200	0.43265300	0.00786900
N	-2.19146400	0.50864200	0.00703000
C	-2.63951800	-0.77447100	-0.00037900
C	0.18298600	1.44145900	0.00252600
N	1.45750200	0.82735100	-0.00441200
C	1.68778000	-0.52978700	-0.00258100
N	0.74915700	-1.42726500	0.00726500
O	0.06600600	2.65745900	-0.00311800
N	3.00644400	-0.91760300	-0.06622700
H	-2.73972800	1.35159100	0.00914200
H	2.23151000	1.47124400	-0.07394300
H	3.69181100	-0.33561000	0.38651500
H	3.13467400	-1.90524700	0.08630600
H	-3.69139200	-1.00899200	-0.00258400

aug-cc-pVDZ basis

THE NUCLEAR REPULSION ENERGY = 596.53585162 a.u.

FINAL SCF ENERGY IS = -539.47863789 a.u.

SECOND ORDER CORRELATION ENERGY = -1.80315111 a.u.

FINAL TARGET STATE ENERGY = -541.26929302 a.u.

aug-cc-pVTZ basis

THE NUCLEAR REPULSION ENERGY = 596.53585162 a.u.

FINAL SCF ENERGY IS = -539.56223446 a.u.

SECOND ORDER CORRELATION ENERGY = -2.03450705 a.u.

FINAL TARGET STATE ENERGY = -541.58578149 a.u.

Thyamine

Cartesian Coordinate

N -0.72657200 1.02871800 0.00000200
C 0.66975000 0.89548300 -0.00000100
C 1.15370600 -0.48647800 -0.00000200
C 0.24041000 -1.47495700 -0.00000200
N -1.11528600 -1.23910400 -0.00000100
C -1.67527100 0.02607500 0.00000100
O 1.37803600 1.88423000 -0.00000300
C 2.63232900 -0.71677600 0.00000400
O -2.87224800 0.22291100 0.00000200
H 3.09673900 -0.25874200 0.87432100
H 3.09677000 -0.25853700 -0.87418800
H 2.86355700 -1.78120100 -0.00011500
H 0.52231700 -2.51859800 -0.00000400
H -1.77299000 -2.00033900 -0.00000500
H -1.08523500 1.97290400 0.00000300

aug-cc-pVDZ basis

THE NUCLEAR REPULSION ENERGY = 418.39228582 a.u.

FINAL SCF ENERGY IS = -414.35962309 a.u.

SECOND ORDER CORRELATION ENERGY = -1.37883759 a.u.

FINAL TARGET STATE ENERGY = -415.72790867 a.u.

aug-cc-pVTZ basis

THE NUCLEAR REPULSION ENERGY = 418.39228582 a.u.

FINAL SCF ENERGY IS = -414.08420055 a.u.

SECOND ORDER CORRELATION ENERGY = -1.54315678 a.u.

FINAL TARGET STATE ENERGY = -415.61861271a.u.

Cytosin

Cartesian Coordinate

N -0.72657200 1.02871800 0.00000200
C 0.66975000 0.89548300 -0.00000100
C 1.15370600 -0.48647800 -0.00000200
C 0.24041000 -1.47495700 -0.00000200
N -1.11528600 -1.23910400 -0.00000100
C -1.67527100 0.02607500 0.00000100
O 1.37803600 1.88423000 -0.00000300
C 2.63232900 -0.71677600 0.00000400
O -2.87224800 0.22291100 0.00000200
H 3.09673900 -0.25874200 0.87432100
H 3.09677000 -0.25853700 -0.87418800
H 2.86355700 -1.78120100 -0.00011500
H 0.52231700 -2.51859800 -0.00000400
H -1.77299000 -2.00033900 -0.00000500
H -1.08523500 1.97290400 0.00000300

aug-cc-pVDZ basis

THE NUCLEAR REPULSION ENERGY = 357.45266236 a.u.

FINAL SCF ENERGY IS = -392.68202412 a.u.

SECOND ORDER CORRELATION ENERGY = -1.30444015 a.u.

FINAL TARGET STATE ENERGY = -393.96953879 a.u.

aug-cc-pVTZ basis

THE NUCLEAR REPULSION ENERGY = 357.45266236 a.u.

FINAL SCF ENERGY IS = -392.74423046 a.u.

SECOND ORDER CORRELATION ENERGY = -1.47118070 a.u.

FINAL TARGET STATE ENERGY = -392.71303519 a.u.

N₂

Cartesian Coordinate

N	0.0000	0.0000	0.5488
N	0.0000	0.0000	-0.5488

H₂O

Cartesian Coordinate

O	0.0000	0.0000	0.1173
H	0.0000	0.7572	-0.4692
H	0.0000	-0.7572	-0.4692

CH⁺

Cartesian Coordinate

C	0.0000	0.0000	0.0000
H	0.0000	0.0000	2.1371

F₂

Cartesian Coordinate

F	0.0000	0.0000	0.0000
F	0.0000	0.0000	1.4119

C₂

Cartesian Coordinate

C	0.0000	0.0000	0.0000
C	0.0000	0.0000	1.2425

CO

Cartesian Coordinate

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.1282

NH

Cartesian Coordinate

N	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.0362

NO⁺

Cartesian Coordinate

O	0.0000	0.0000	0.0000
N	0.0000	0.0000	1.1508

O₂

Cartesian Coordinate

O	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.2075

BH

Cartesian Coordinate

B	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.2324

O₃

Cartesian Coordinate

O	0.0000	0.0000	0.0000
O	0.0000	1.0885	0.6697
O	0.0000	-1.0885	0.6697

C₂H₂

Cartesian Coordinate

C	0.0000	0.0000	0.6013
C	0.0000	0.0000	-0.6013
H	0.0000	0.0000	1.6644
H	0.0000	0.0000	-1.6644

C₂H₄

Cartesian Coordinate

C	0.0000	0.0000	0.6695
C	0.0000	0.0000	-0.6695
H	0.0000	0.9289	1.2321
H	0.0000	-0.9289	1.2321
H	0.0000	0.9289	-1.2321
H	0.0000	-0.9289	-1.2321

CO₂

Cartesian Coordinate

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.1621
O	0.0000	0.0000	-1.1621

LiF

Cartesian Coordinate

F	0.0000	0.0000	0.0000
Li	0.0000	0.0000	1.5639

NaH

Cartesian Coordinate

Na	0.0000	0.0000	0.0000
H	0.0000	0.0000	1.8874

BeO

Cartesian Coordinate

Be	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.3309

Cl₂

Cartesian Coordinate

Cl	0.0000	0.0000	0.0000
Cl	0.0000	0.0000	1.9879

H₂S

Cartesian Coordinate

S	0.0000	0.0000	0.0000
H	0.0000	0.9569	0.9208
H	0.0000	-0.9569	0.9208

H₂CO

Cartesian Coordinate

O	0.0000	0.0000	1.2050
C	0.0000	0.0000	0.0000
H	0.0000	0.9429	-0.5876
H	0.0000	-0.9429	-0.5876

Table S1: Electron affinities of N₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-2.64	-2.66	-2.64	-2.65
	2	-2.69	-2.86	-2.68	-2.85
	3	-2.69	-2.86	-2.68	-2.85
	4	-3.15	-3.18	-3.15	-3.18
	5	-3.78	-3.80	-3.79	-3.80
aug-cc- pVTZ	1	-2.08	-2.07	-2.06	-2.07
	2	-2.26	-2.28	-2.26	-2.27
	3	-2.46	-2.58	-2.43	-2.54
	4	-2.46	-2.58	-2.43	-2.54
	5	-2.94	-2.95	-2.94	-2.95
aug-cc- pVQZ	1	-1.70	-1.70	-1.69	-1.70
	2	-1.70	-1.71	-1.70	-1.71
	3	-2.33	-2.41	-2.29	-2.37
	4	-2.33	-2.41	-2.29	-2.37
	5	-2.41	-2.41	-2.41	-2.41

Table S2: Electron affinities of H₂O (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-0.78	-0.80	-0.77	-0.80
	2	-1.50	-1.51	-1.50	-1.52
	3	-4.36	-4.40	-4.38	-4.43
	4	-5.17	-5.20	-5.20	-5.24
	5	-5.54	-5.61	-5.57	-5.64
aug-cc- pVTZ	1	-0.62	-0.64	-0.63	-0.64
	2	-1.23	-1.24	-1.24	-1.24
	3	-3.26	-3.28	-3.27	-3.30
	4	-4.04	-4.06	-4.06	-4.08
	5	-4.20	-4.24	-4.22	-4.26
aug-cc- pVQZ	1	-0.54	-0.56	-0.55	-0.56
	2	-1.10	-1.11	-1.11	-1.11
	3	-2.70	-2.71	-2.71	-2.72
	4	-3.29	-3.30	-3.30	-3.32
	5	-3.45	-3.48	-3.45	-3.49

Table S3: Electron affinities of CH⁺ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	10.41	10.06	10.73	10.35
	2	10.41	10.06	10.73	10.35
	3	4.08	4.01	4.13	4.05
	4	2.02	1.97	2.03	1.97
	5	2.05	1.93	2.10	1.95
aug-cc- pVTZ	1	10.56	10.28	10.91	10.60
	2	10.56	10.28	10.91	10.60
	3	4.12	4.07	4.17	4.11
	4	2.32	2.28	2.35	2.29
	5	2.26	2.17	2.30	2.19
aug-cc- pVQZ	1	10.60	10.35	10.96	10.68
	2	10.60	10.35	10.96	10.68
	3	4.13	4.08	4.19	4.12
	4	2.45	2.41	2.48	2.43
	5	2.36	2.29	2.40	2.31

Table S4: Electron affinities of F₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	0.01	-0.23	-0.16	-0.38
	2	-4.81	-4.91	-4.87	-4.97
	3	-4.91	-4.94	-4.95	-4.99
	4	-6.16	-6.18	-6.18	-6.21
	5	-6.16	-6.18	-6.18	-6.21
aug-cc- pVTZ	1	0.06	-0.08	-0.03	-0.17
	2	-3.70	-3.73	-3.73	-3.76
	3	-3.84	-3.89	-3.88	-3.93
	4	-4.83	-4.84	-4.84	-4.86
	5	-4.83	-4.84	-4.84	-4.86
aug-cc- pVQZ	1	0.16	0.05	0.08	-0.02
	2	-2.67	-2.69	-2.69	-2.70
	3	-3.10	-3.14	-3.13	-3.16
	4	-3.93	-3.95	-3.94	-3.95
	5	-3.93	-3.95	-3.94	-3.95

Table S5: Electron affinities of C₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	3.21	3.15	3.65	3.58
	2	-1.64	-1.61	-1.63	-1.62
	3	-2.28	-2.31	-2.26	-2.31
	4	-2.45	-2.50	-2.43	-2.49
	5	-2.45	-2.50	-2.43	-2.49
aug-cc- pVTZ	1	3.39	3.41	3.83	3.83
	2	-1.31	-1.29	-1.31	-1.30
	3	-1.64	-1.65	-1.63	-1.65
	4	-2.24	-2.23	-2.23	-2.23
	5	-2.24	-2.23	-2.23	-2.23
aug-cc- pVQZ	1	3.44	3.50	3.89	3.93
	2	-1.10	-1.08	-1.10	-1.08
	3	-1.27	-1.27	-1.26	-1.26
	4	-1.84	-1.84	-1.84	-1.84
	5	-1.84	-1.84	-1.84	-1.84

Table S6: Electron affinities of CO (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-1.78	-1.87	-1.75	-1.85
	2	-1.78	-1.87	-1.75	-1.85
	3	-1.98	-2.01	-2.01	-2.03
	4	-2.54	-2.57	-2.50	-2.53
	5	-3.65	-3.83	-3.57	-3.76
aug-cc- pVTZ	1	-1.55	-1.61	-1.52	-1.58
	2	-1.55	-1.61	-1.52	-1.58
	3	-1.62	-1.63	-1.62	-1.63
	4	-1.91	-1.93	-1.91	-1.92
	5	-2.98	-3.11	-2.90	-3.03
aug-cc- pVQZ	1	-1.29	-1.30	-1.26	-1.27
	2	-1.54	-1.55	-1.37	-1.41
	3	-1.55	-1.56	-1.37	-1.41
	4	-1.61	-1.61	-1.60	-1.61
	5	-2.60	-3.23	-2.51	-2.62

Table S7: Electron affinities of NH (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	2.02	1.43	2.33	1.72
	2	-0.84	-0.87	-0.83	-0.87
	3				
		-3.76	-3.97	-3.90	-3.98
	4	-3.92	-4.39	-4.39	-4.38
	5	-4.41	-4.46	-4.63	-4.47
aug-cc- pVTZ	1	2.09	1.61	2.45	1.94
	2	-0.68	-0.70	-0.67	-0.69
	3				
		-2.92	-2.94	-2.92	-2.95
	4	-3.00	-3.37	-3.36	-3.34
	5	-3.36	-3.40	-3.54	-3.40
aug-cc- pVQZ	1	2.12	1.69	2.5	2.04
	2	-0.59	-0.60	-0.58	-0.60
	3				
		-2.29	-2.31	-2.29	-2.31
	4	-2.47	-2.72	-2.72	-2.70
	5	-2.73	-2.75	-2.83	-2.75

Table S8: Electron affinities of NO⁺ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	9.38	9.25	9.39	9.25
	2	9.38	9.25	9.39	9.25
	3	3.33	3.31	3.31	3.29
	4	2.10	2.10	2.14	2.12
	5	1.91	1.91	1.92	1.92
aug-cc- pVTZ	1	9.65	9.59	9.66	9.60
	2	9.65	9.59	9.66	9.60
	3	3.52	3.51	3.51	3.50
	4	2.39	2.39	2.41	2.40
	5	2.24	2.25	2.25	2.26
aug-cc- pVQZ	1	9.74	9.72	9.77	9.74
	2	9.74	9.72	9.77	9.74
	3	3.65	3.65	3.65	3.65
	4	2.54	2.54	2.55	2.55
	5	2.43	2.44	2.43	2.44

Table S9: Electron affinities of O₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	0.77	0.50	0.70	0.44
	2	-3.05	-3.07	-3.06	-3.08
	3				
		-3.93	-3.95	-3.95	-3.98
	4	-4.57	-4.60	-4.60	-4.63
	5	-4.93	-4.95	-4.93	-4.96
aug-cc- pVTZ	1	0.93	0.74	0.91	0.73
	2	-2.51	-2.51	-2.51	-2.52
	3				
		-2.92	-2.93	-2.93	-2.94
	4	-3.60	-3.61	-3.62	-3.62
	5	-3.83	-3.84	-3.83	-3.84
aug-cc- pVQZ	1	1.01	0.87	1.00	0.87
	2	-2.06	-2.06	-2.06	-2.07
	3				
		-2.14	-2.14	-2.14	-2.15
	4	-2.95	-2.96	-2.97	-2.97
	5	-3.13	-3.14	-3.13	-3.14

Table S10: Electron affinities of BH (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	10.38	10.04	10.71	10.32
	2	10.38	10.04	10.71	10.32
	3				
		4.29	4.19	4.37	4.26
	4	2.08	2.01	2.11	2.03
	5	2.06	1.93	2.05	1.95
aug-cc- pVTZ	1	10.53	10.25	10.88	10.57
	2	10.53	10.25	10.88	10.57
	3				
		4.35	4.27	4.43	4.34
	4	2.42	2.36	2.47	2.39
	5	2.26	2.17	2.31	2.19
aug-cc- pVQZ	1	10.57	10.32	10.94	10.66
	2	10.57	10.32	10.94	10.66
	3				
		4.36	4.29	4.45	4.36
	4	2.56	2.51	2.60	2.54
	5	2.37	2.30	2.41	2.32

Table S11: Electron affinities of O₃ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	1.62	1.58	1.18	1.16
	2	-3.05	-3.03	-3.09	-3.08
	3	-3.07	-3.03	-3.10	-3.09
	4	-3.43	-3.41	-3.46	-3.46
	5	-4.47	-4.48	-4.53	-4.54
aug-cc- pVTZ	1	1.84	1.88	1.42	1.49
	2	-2.47	-2.45	-2.50	-2.49
	3	-2.55	-2.53	-2.55	-2.54
	4	-2.59	-2.55	-2.63	-2.60
	5	-3.49	-3.48	-3.52	-3.52
aug-cc- pVQZ	1	1.94	2.03	1.53	1.65
	2	-1.91	-1.89	-1.92	-1.90
	3	-2.01	-1.99	-2.03	-2.01
	4	-2.14	-2.12	-2.14	-2.13
	5	-2.85	-2.85	-2.88	-2.87

Table S12: Electron affinities of C₂H₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-0.86	-0.88	-0.86	-0.87
	2	-0.96	-0.97	-0.95	-0.96
	3	-2.53	-2.60	-2.49	-2.56
	4	-2.53	-2.60	-2.49	-2.56
	5	-2.99	-3.01	-3.00	-3.02
aug-cc- pVTZ	1	-0.68	-0.69	-0.67	-0.68
	2	-0.79	-0.80	-0.79	-0.79
	3	-2.21	-2.24	-2.18	-2.21
	4	-2.21	-2.24	-2.18	-2.21
	5	-2.30	-2.31	-2.30	-2.31
aug-cc- pVQZ	1	-0.56	-0.57	-0.55	-0.56
	2	-0.69	-0.70	-0.68	-0.69
	3	-1.88	-1.89	-1.88	-1.89
	4	-1.88	-1.89	-1.88	-1.89
	5	-1.95	-1.95	-1.92	-1.93

TableS13: Electron affinities of C₂H₄ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-0.89	-0.92	-0.88	-0.91
	2	-1.22	-1.24	-1.21	-1.23
	3				
		-1.27	-1.28	-1.26	-1.28
	4	-1.86	-1.87	-1.85	-1.87
	5	-2.07	-2.17	-1.98	-2.09
aug-cc- pVTZ	1	-0.70	-0.71	-0.69	-0.71
	2	-0.98	-0.99	-0.97	-0.99
	3				
		-1.04	-1.05	-1.03	-1.04
	4	-1.57	-1.58	-1.56	-1.57
	5	-1.89	-1.94	-1.78	-1.84
aug-cc- pVQZ	1	-0.60	-0.61	-0.59	-0.60
	2	-0.86	-0.87	-0.86	-0.87
	3				
		-0.93	-0.94	-0.92	-0.93
	4	-1.36	-1.37	-1.36	-1.37
	5	-1.78	-1.80	-1.68	-1.71

Table S14: Electron affinities of CO₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-1.05	-1.07	-1.04	-1.07
	2	-2.22	-2.23	-2.21	-2.23
	3				
		-2.22	-2.23	-2.21	-2.23
	4	-2.33	-2.34	-2.35	-2.37
	5	-4.51	-4.48	-4.42	-4.54
aug-cc- pVTZ	1	-0.89	-0.90	-0.88	-0.89
	2	-1.85	-1.86	-1.85	-1.85
	3				
		-1.85	-1.86	-1.85	-1.85
	4	-1.94	-1.94	-1.95	-1.96
	5	-3.29	-3.29	-3.29	-3.30
aug-cc- pVQZ	1	-0.78	-0.78	-0.77	-0.77
	2	-1.58	-1.58	-1.58	-1.58
	3				
		-1.58	-1.58	-1.58	-1.58
	4	-1.58	-1.59	-1.60	-1.60
	5	-2.69	-2.70	-2.70	-2.71

Table S15: Electron affinities of LIF (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	0.33	0.33	0.34	0.33
	2	-0.34	-0.34	-0.34	-0.34
	3	-0.34	-0.34	-0.34	-0.34
	4	-0.46	-0.46	-0.46	-0.46
	5	-0.85	-0.85	-0.85	-0.85
aug-cc- pVTZ	1	0.33	0.32	0.34	0.33
	2	-0.44	-0.44	-0.44	-0.44
	3	-0.44	-0.44	-0.44	-0.44
	4	-0.55	-0.56	-0.55	-0.56
	5	-0.73	-0.74	-0.74	-0.74
aug-cc- pVQZ	1	0.34	0.33	0.34	0.33
	2	-0.35	-0.35	-0.35	-0.35
	3	-0.35	-0.35	-0.35	-0.35
	4	-0.38	-0.38	-0.38	-0.38
	5	-0.56	-0.56	-0.56	-0.57

Table S16: Electron affinities of NaH (in eV)

Basis	State	EOMEA- CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	0.31	0.29	0.34	0.31
	2	-0.31	-0.32	-0.31	-0.32
	3	-0.31	-0.32	-0.31	-0.32
	4	-0.50	-0.52	-0.49	-0.50
	5	-0.69	-0.71	-0.70	-0.71
aug-cc- pVTZ	1	0.32	0.30	0.35	0.32
	2	-0.28	-0.28	-0.27	-0.28
	3	-0.28	-0.28	-0.27	-0.28
	4	-0.37	-0.38	-0.36	-0.37
	5	-0.53	-0.54	-0.54	-0.54
aug-cc- pVQZ	1	0.32	0.30	0.35	0.33
	2	-0.23	-0.23	-0.22	-0.23
	3	-0.27	-0.27	-0.26	-0.27
	4	-0.27	-0.27	-0.26	-0.27
	5	-0.47	-0.48	-0.47	-0.47

Table S17: Electron affinities of Cl₂ (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	0.50	0.37	0.57	0.43
	2	-2.43	-2.48	-2.43	-2.48
	3				
		-2.68	-2.75	-2.67	-2.74
	4	-3.31	-3.35	-3.31	-3.35
	5	-3.31	-3.35	-3.31	-3.35
aug-cc- pVTZ	1	0.55	0.49	0.68	0.61
	2	-1.86	-1.89	-1.86	-1.88
	3				
		-2.17	-2.20	-2.15	-2.19
	4	-2.55	-2.57	-2.55	-2.57
	5	-2.55	-2.57	-2.55	-2.57
aug-cc- pVQZ	1	0.66	0.65	0.80	0.77
	2	-1.19	-1.20	-1.18	-1.20
	3				
		-1.69	-1.70	-1.67	-1.69
	4	-2.13	-2.14	-2.12	-2.14
	5	-2.13	-2.14	-2.12	-2.14

Table S18: Electron affinities of BeO (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	2.11	2.12	2.22	2.19
	2	-0.47	-0.47	-0.44	-0.45
	3	-0.49	-0.49	-0.48	-0.49
	4	-0.49	-0.49	-0.48	-0.49
	5	-1.24	-1.24	-1.24	-1.25
aug-cc- pVTZ	1	2.13	2.16	2.23	2.23
	2	-0.32	-0.32	-0.30	-0.30
	3	-0.40	-0.40	-0.40	-0.40
	4	-0.40	-0.40	-0.40	-0.40
	5	-0.90	-0.90	-0.91	-0.92
aug-cc- pVQZ	1	2.15	2.18	2.25	2.25
	2	-0.27	-0.27	-0.25	-0.25
	3	-0.36	-0.36	-0.36	-0.36
	4	-0.36	-0.36	-0.36	-0.36
	5	-0.79	-0.79	-0.80	-0.80

Table S19: Electron affinities of H₂S (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-0.66	-0.70	-0.65	-0.69
	2	-1.53	-1.56	-1.52	-1.55
	3				
		-2.71	-2.74	-2.71	-2.74
	4	-2.83	-2.91	-2.78	-2.87
	5	-3.19	-3.22	-3.18	-3.22
aug-cc- pVTZ	1	-0.53	-0.55	-0.51	-0.54
	2	-1.23	-1.24	-1.22	-1.23
	3				
		-2.08	-2.09	-2.07	-2.09
	4	-2.32	-2.33	-2.31	-2.33
	5	-2.43	-2.48	-2.38	-2.44
aug-cc- pVQZ	1	-0.43	-0.45	-0.42	-0.43
	2	-1.09	-1.10	-1.08	-1.10
	3				
		-1.65	-1.67	-1.65	-1.66
	4	-1.82	-1.83	-1.81	-1.83
	5	-2.11	-2.14	-2.07	-2.10

Table S20: Electron affinities of H₂CO (in eV)

Basis	State	EOMEA-CCSD	P-EOMEA- CCSD	EOMEA- CCSD(2)	P-EOMEA- CCSD(2)
aug-cc- pVDZ	1	-0.75	-0.77	-0.73	-0.75
	2	-1.25	-1.32	-1.24	-1.31
	3	-1.31	-1.36	-1.29	-1.35
	4	-2.19	-2.22	-2.21	-2.24
	5	-3.10	-3.19	-3.08	-3.17
aug-cc- pVTZ	1	-0.59	-0.60	-0.56	-0.58
	2	-1.07	-1.08	-1.05	-1.06
	3	-1.08	-1.14	-1.05	-1.12
	4	-1.85	-1.87	-1.86	-1.88
	5	-2.48	-2.53	-2.44	-2.50
aug-cc- pVQZ	1	-0.50	-0.50	-0.48	-0.49
	2	-0.96	-0.97	-0.95	-0.96
	3	-0.99	-1.03	-0.96	-1.00
	4	-1.58	-1.59	-1.59	-1.60
	5	-2.11	-2.14	-2.07	-2.11

