Supplementary Information

Variational formulation of perturbative explicitly correlated coupled cluster methods.

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TABLE I: Experimental geometries for the test molecules. Taken from Ref. 1. Bond lengths are given in Å and bond angles in degree.

molecule	internal coordinate	value[1,2]
H_2	R_{HH}	0.74144
HF	R_{HF}	0.91680(8)
H_2O	R_{OH}	0.9572
	$\angle_{HOH}$	104.52
HOF	R_{OH}	0.9657
	R_{FO}	1.4350(31)
	$\angle_{HOF}$	97.54(50)
H_2O_2	R_{OH}	0.967
	R_{OO}	1.4556
	$\angle_{HOO}$	102.32
	$\angle_{HOOH}$	113.70[3]
HNC	R_{NH}	0.9940(8)
	R_{CN}	1.1689(2)
NH_3	R_{NH}	1.011(6)
	$\angle_{HNH}$	106.7
N_2H_2	R_{NH}	1.029(1)
	R_{NN}	1.247(1)
	$\angle_{HNN}$	106.3(2)
C_2H_2	R_{CH}	1.06215(17)
	R_{CC}	1.20257(9)
HNO	R_{NH} (R_0)	1.062(8)
	R_{NO} (R_0)	1.211(6)
	$\angle_{HNO}$ (θ_0)	108.5(8)
HCN	R_{CH}	1.06501(8)
	R_{CN}	1.15324(2)
C_2H_4	R_{CH}	1.081(2)
	R_{CC}	1.334(2)
	$\angle_{HCH}$	117.37(33)
CH_4	R_{CH}	1.0858(10)
N_2	R_{NN}	1.09768(5)
CH_2O	R_{CH}	1.1005(20)
	R_{CO}	1.2033(10)
	$\angle_{HCH}$	116.30(25)
CH_2	R_{CH}	1.107(2)
	$\angle_{HCH}$	102.4(4)
CO	R_{CO}	1.12832
CO_2	R_{CO}	1.15995
O_3	R_{OO}	1.2717(2)
	$\angle_{OOO}$	116.78(33)
F_2	R_{FF}	1.41193

[1] Bond lengths from table 15.3 of [1].
[2] Bond angles from table 15.8 of [1].
[3] Dihedral from original literature as cited below table 15.3 of [1].

TABLE IV: The valence correlation contributions to the electronic reaction energies, $\Delta H_e^0(0\mathrm{K})$, (in kJ/mol) for the 12 test reactions[1].

		CCSD(T)		CCSD(T)$_{\overline{R12}}$			
				d			
		E	Δ_{CBS}[2]	E	Δ_{CBS}[2]	E	Δ_{CBS}[2]
1	aug-cc-pVDZ	−11.86	11.98	−20.41	3.43	−21.12	2.72
	aug-cc-pVTZ	−22.22	1.62	−23.96	−0.12	−23.86	−0.02
	CBS	−23.84		−23.84		−23.84	
2	aug-cc-pVDZ	3.07	19.02	−13.62	2.33	−13.98	1.98
	aug-cc-pVTZ	−14.42	1.53	−17.60	−1.65	−17.11	−1.16
	CBS	−15.95		−15.95		−15.95	
3	aug-cc-pVDZ	5.12	−2.23	4.35	−3.00	4.92	−2.43
	aug-cc-pVTZ	6.35	−1.00	7.24	−0.11	7.23	−0.12
	CBS	7.35		7.35		7.35	
4	aug-cc-pVDZ	13.72	15.43	−1.55	0.16	−2.03	−0.33
	aug-cc-pVTZ	−3.26	−1.55	−2.94	−1.24	−2.42	−0.71
	CBS	−1.71		−1.71		−1.71	
5	aug-cc-pVDZ	7.33	10.17	−1.81	1.03	−2.17	0.68
	aug-cc-pVTZ	−2.53	0.31	−3.34	−0.50	−3.08	−0.24
	CBS	−2.84		−2.84		−2.84	
6	aug-cc-pVDZ	−4.53	22.15	−22.22	4.46	−23.29	3.40
	aug-cc-pVTZ	−24.75	1.93	−27.30	−0.62	−26.94	−0.26
	CBS	−26.69		−26.69		−26.69	
7	aug-cc-pVDZ	21.50	12.51	8.54	−0.45	8.21	−0.79
	aug-cc-pVTZ	8.89	−0.10	8.14	−0.86	8.38	−0.62
	CBS	8.99		8.99		8.99	
8	aug-cc-pVDZ	34.98	15.88	20.19	1.09	20.75	1.65
	aug-cc-pVTZ	22.80	3.71	18.30	−0.79	18.91	−0.18
	CBS	19.10		19.10		19.10	
9	aug-cc-pVDZ	19.91	0.61	15.48	−3.82	16.37	−2.93
	aug-cc-pVTZ	16.51	−2.79	18.04	−1.26	18.14	−1.16
	CBS	19.30		19.30		19.30	
10	aug-cc-pVDZ	−33.94	13.28	−45.38	1.84	−45.76	1.46
	aug-cc-pVTZ	−43.11	4.11	−46.88	0.35	−46.71	0.51
	CBS	−47.22		−47.22		−47.22	
11	aug-cc-pVDZ	62.80	12.04	48.44	−2.32	50.37	−0.39
	aug-cc-pVTZ	56.61	5.86	50.24	−0.52	51.28	0.53
	CBS	50.75		50.75		50.75	
12	aug-cc-pVDZ	−82.68	23.72	−101.89	4.50	−102.97	3.42
	aug-cc-pVTZ	−96.38	10.01	−104.55	1.85	−104.32	2.07
	CBS	−106.39		−106.39		−106.39	

[1] See Table V in the main text.

[2] The difference between the respective reaction energy correlation contribution and the associated CBS value. The CBS value was obtained by Schwenke extrapolation[2] using the aug-cc-pVQZ and aug-cc-pV5Z basis sets. The CCSD correlation energy and the (T) correction were extrapolated separately.

TABLE II: The valence correlation energies (in mE_h) of the 20 test molecules. CBS refers to the correlation energy obtained by the basis set extrapolation with Schwenke method[2] using aug-cc-pVQZ and aug-cc-pV5Z basis sets.

		CCSD		CCSD(2)$_{\overline{R12}}$			
				d			
	basis set	E	%	E	%	E	%
H_2	aug-cc-pVDZ	−35.83	87.7	−39.97	97.8	−39.99	97.8
	aug-cc-pVTZ	−39.61	96.9	−40.62	99.4	−40.68	99.5
	CBS	−40.88		−40.88		−40.88	
CH_2	aug-cc-pVDZ	−143.22	81.5	−168.70	96.0	−169.83	96.7
	aug-cc-pVTZ	−166.10	94.6	−174.29	99.2	−174.56	99.4
	CBS	−175.64		−175.64		−175.64	
CH_4	aug-cc-pVDZ	−191.03	82.0	−225.01	96.6	−226.30	97.2
	aug-cc-pVTZ	−220.69	94.7	−231.32	99.3	−231.59	99.4
	CBS	−232.93		−232.93		−232.93	
H_2O	aug-cc-pVDZ	−227.11	76.2	−290.27	97.4	−291.51	97.8
	aug-cc-pVTZ	−273.05	91.6	−294.73	98.9	−295.42	99.1
	CBS	−298.09		−298.09		−298.09	
NH_3	aug-cc-pVDZ	−214.32	79.5	−261.00	96.9	−262.32	97.3
	aug-cc-pVTZ	−251.86	93.5	−267.24	99.2	−267.64	99.3
	CBS	−269.47		−269.47		−269.47	
HF	aug-cc-pVDZ	−225.97	72.0	−307.61	98.0	−308.81	98.4
	aug-cc-pVTZ	−280.97	89.5	−309.10	98.5	−310.33	98.9
	CBS	−313.90		−313.90		−313.90	
N_2	aug-cc-pVDZ	−319.81	78.5	−394.39	96.8	−396.84	97.4
	aug-cc-pVTZ	−376.88	92.5	−403.42	99.0	−404.21	99.2
	CBS	−407.57		−407.57		−407.57	
F_2	aug-cc-pVDZ	−435.45	72.5	−589.12	98.0	−592.25	98.5
	aug-cc-pVTZ	−538.96	89.7	−591.79	98.5	−594.59	98.9
	CBS	−601.00		−601.00		−601.00	
CO	aug-cc-pVDZ	−306.29	77.4	−384.26	97.1	−386.34	97.6
	aug-cc-pVTZ	−363.09	91.7	−391.40	98.9	−392.31	99.1
	CBS	−395.75		−395.75		−395.75	
HCN	aug-cc-pVDZ	−302.63	79.8	−365.92	96.4	−368.36	97.1
	aug-cc-pVTZ	−353.51	93.2	−376.22	99.2	−376.80	99.3
	CBS	−379.43		−379.43		−379.43	
HNC	aug-cc-pVDZ	−295.73	79.5	−359.09	96.6	−361.42	97.2
	aug-cc-pVTZ	−346.00	93.1	−368.52	99.1	−369.07	99.3
	CBS	−371.76		−371.76		−371.76	
C_2H_2	aug-cc-pVDZ	−278.86	80.5	−332.70	96.0	−335.58	96.8
	aug-cc-pVTZ	−325.04	93.8	−343.87	99.2	−344.25	99.3
	CBS	−346.59		−346.59		−346.59	
C_2H_4	aug-cc-pVDZ	−313.83	81.3	−372.11	96.4	−374.79	97.1
	aug-cc-pVTZ	−363.58	94.2	−383.07	99.2	−383.52	99.3
	CBS	−386.07		−386.07		−386.07	
CH_2O	aug-cc-pVDZ	−347.02	77.8	−432.39	97.0	−434.76	97.5
	aug-cc-pVTZ	−411.35	92.3	−441.33	99.0	−442.27	99.2
	CBS	−445.85		−445.85		−445.85	
HNO	aug-cc-pVDZ	−379.09	77.6	−475.01	97.2	−477.76	97.8
	aug-cc-pVTZ	−450.22	92.1	−483.55	98.9	−484.75	99.2
	CBS	−488.71		−488.71		−488.71	
N_2H_2	aug-cc-pVDZ	−363.11	79.1	−444.16	96.8	−446.94	97.4
	aug-cc-pVTZ	−426.85	93.0	−454.64	99.1	−455.48	99.3
	CBS	−458.83		−458.83		−458.83	
HOF	aug-cc-pVDZ	−428.91	74.1	−565.84	97.7	−568.91	98.2
	aug-cc-pVTZ	−524.15	90.5	−571.37	98.7	−573.52	99.0
	CBS	−579.14		−579.14		−579.14	
H_2O_2	aug-cc-pVDZ	−428.48	76.2	−547.97	97.4	−551.05	98.0
	aug-cc-pVTZ	−514.97	91.6	−556.16	98.9	−557.70	99.2
	CBS	−562.45		−562.45		−562.45	
CO_2	aug-cc-pVDZ	−501.12	76.1	−639.02	97.0	−642.55	97.5
	aug-cc-pVTZ	−601.18	91.2	−651.26	98.8	−652.86	99.1
	CBS	−658.84		−658.84		−658.84	
O_3	aug-cc-pVDZ	−640.95	77.6	−807.34	97.7	−812.12	98.3
	aug-cc-pVTZ	−759.04	91.9	−816.82	98.9	−819.33	99.2
	CBS	−825.94		−825.94		−825.94	

TABLE III: The valence correlation energies (in mE_h) of the 20 test molecules. CBS refers to the correlation energy obtained by basis set extrapolation with Schwenke method[2] using aug-cc-pVQZ and aug-cc-pV5Z basis sets. The CCSD correlation energy and the (T) energy correction were extrapolated separately.

		CCSD(T)		CCSD(T)$_{\overline{R12}}$			
				d			
	basis set	E	%	E	%	E	%
H_2	aug-cc-pVDZ	−35.83	87.7	−39.97	97.8	−39.99	97.8
	aug-cc-pVTZ	−39.61	96.9	−40.62	99.4	−40.68	99.5
	CBS	−40.88		−40.88		−40.88	
CH_2	aug-cc-pVDZ	−146.74	80.9	−172.22	95.0	−173.35	95.6
	aug-cc-pVTZ	−171.19	94.4	−179.38	98.9	−179.65	99.1
	CBS	−181.31		−181.31		−181.31	
CH_4	aug-cc-pVDZ	−195.50	81.4	−229.47	95.5	−230.77	96.1
	aug-cc-pVTZ	−227.22	94.6	−237.85	99.0	−238.12	99.1
	CBS	−240.17		−240.17		−240.17	
H_2O	aug-cc-pVDZ	−232.31	75.4	−295.47	95.9	−296.71	96.3
	aug-cc-pVTZ	−281.68	91.5	−303.35	98.5	−304.04	98.7
	CBS	−307.96		−307.96		−307.96	
NH_3	aug-cc-pVDZ	−219.77	78.8	−266.46	95.6	−267.77	96.0
	aug-cc-pVTZ	−260.19	93.3	−275.57	98.8	−275.97	99.0
	CBS	−278.79		−278.79		−278.79	
HF	aug-cc-pVDZ	−230.11	71.3	−311.75	96.6	−312.95	97.0
	aug-cc-pVTZ	−288.48	89.4	−316.61	98.1	−317.84	98.5
	CBS	−322.74		−322.74		−322.74	
N_2	aug-cc-pVDZ	−333.22	77.7	−407.80	95.1	−410.26	95.7
	aug-cc-pVTZ	−396.04	92.3	−422.58	98.5	−423.38	98.7
	CBS	−428.88		−428.88		−428.88	
F_2	aug-cc-pVDZ	−448.31	71.9	−601.97	96.5	−605.10	97.0
	aug-cc-pVTZ	−558.91	89.6	−611.75	98.0	−614.54	98.5
	CBS	−623.94		−623.94		−623.94	
CO	aug-cc-pVDZ	−318.59	76.7	−396.56	95.5	−398.64	96.0
	aug-cc-pVTZ	−380.63	91.6	−408.95	98.5	−409.86	98.7
	CBS	−415.34		−415.34		−415.34	
HCN	aug-cc-pVDZ	−315.97	79.0	−379.26	94.9	−381.70	95.5
	aug-cc-pVTZ	−371.96	93.0	−394.67	98.7	−395.24	98.9
	CBS	−399.76		−399.76		−399.76	
HNC	aug-cc-pVDZ	−308.76	78.9	−372.12	95.1	−374.45	95.7
	aug-cc-pVTZ	−363.90	93.0	−386.42	98.7	−386.97	98.9
	CBS	−391.46		−391.46		−391.46	
C_2H_2	aug-cc-pVDZ	−291.08	79.7	−344.92	94.5	−347.80	95.3
	aug-cc-pVTZ	−341.90	93.7	−360.72	98.8	−361.11	98.9
	CBS	−365.06		−365.06		−365.06	
C_2H_4	aug-cc-pVDZ	−324.97	80.6	−383.24	95.1	−385.92	95.7
	aug-cc-pVTZ	−379.09	94.0	−398.58	98.9	−399.04	99.0
	CBS	−403.14		−403.14		−403.14	
CH_2O	aug-cc-pVDZ	−358.94	77.1	−444.31	95.5	−446.68	96.0
	aug-cc-pVTZ	−428.71	92.1	−458.70	98.6	−459.63	98.8
	CBS	−465.29		−465.29		−465.29	
HNO	aug-cc-pVDZ	−393.75	76.9	−489.67	95.6	−492.41	96.1
	aug-cc-pVTZ	−471.33	92.0	−504.66	98.5	−505.86	98.7
	CBS	−512.27		−512.27		−512.27	
N_2H_2	aug-cc-pVDZ	−377.14	78.4	−458.19	95.3	−460.97	95.8
	aug-cc-pVTZ	−446.77	92.9	−474.57	98.7	−475.40	98.9
	CBS	−480.93		−480.93		−480.93	
HOF	aug-cc-pVDZ	−441.75	73.4	−578.68	96.2	−581.75	96.7
	aug-cc-pVTZ	−544.00	90.4	−591.22	98.2	−593.37	98.6
	CBS	−601.80		−601.80		−601.80	
H_2O_2	aug-cc-pVDZ	−441.63	75.4	−561.12	95.9	−564.19	96.4
	aug-cc-pVTZ	−535.19	91.4	−576.37	98.5	−577.91	98.7
	CBS	−585.36		−585.36		−585.36	
CO_2	aug-cc-pVDZ	−522.03	75.4	−659.93	95.4	−663.46	95.9
	aug-cc-pVTZ	−630.88	91.2	−680.96	98.4	−682.56	98.6
	CBS	−691.93		−691.93		−691.93	
O_3	aug-cc-pVDZ	−678.47	77.1	−844.86	96.0	−849.64	96.6
	aug-cc-pVTZ	−808.38	91.9	−866.16	98.4	−868.67	98.7
	CBS	−879.83		−879.83		−879.83	

TABLE V: The electronic reaction energies, $\Delta H_e^0(0\mathrm{K})$, (in kJ/mol) for the 12 test reactions[1].

		CCSD(T)		CCSD(T)$_{\overline{\mathrm{R12}}}$			
				d			
		E	$\Delta_{\mathrm{experimental}}$ [2]	E	$\Delta_{\mathrm{experimental}}$ [2]	E	$\Delta_{\mathrm{experimental}}$ [2]
1	aug-cc-pVDZ[2]	−18.20	3.6	−26.74	−4.9	−27.46	−5.7
	aug-cc-pVTZ[2]	−22.62	−0.8	−24.37	−2.6	−24.26	−2.5
	experimental[1]	−21.8		−21.8		−21.8	
2	aug-cc-pVDZ[2]	−166.06	−0.7	−182.75	−17.3	−183.11	−17.7
	aug-cc-pVTZ[2]	−165.52	−0.1	−168.69	−3.3	−168.21	−2.8
	experimental[1]	−165.4		−165.4		−165.4	
3	aug-cc-pVDZ[2]	−220.93	−17.0	−221.69	−17.8	−221.13	−17.2
	aug-cc-pVTZ[2]	−206.94	−3.0	−206.05	−2.2	−206.06	−2.2
	experimental[1]	−203.9		−203.9		−203.9	
4	aug-cc-pVDZ[2]	−261.00	−15.7	−276.27	−31.0	−276.76	−31.5
	aug-cc-pVTZ[2]	−248.69	−3.4	−248.37	−3.1	−247.85	−2.5
	experimental[1]	−245.3		−245.3		−245.3	
5	aug-cc-pVDZ[2]	−251.16	0.7	−260.30	−8.4	−260.66	−8.8
	aug-cc-pVTZ[2]	−250.75	1.1	−251.56	0.3	−251.30	0.6
	experimental[1]	−251.9		−251.9		−251.9	
6	aug-cc-pVDZ[2]	−269.36	4.4	−287.05	−13.2	−288.12	−14.3
	aug-cc-pVTZ[2]	−273.37	0.4	−275.92	−2.1	−275.57	−1.8
	experimental[1]	−273.8		−273.8		−273.8	
7	aug-cc-pVDZ[2]	−323.58	−3.3	−336.54	−16.2	−336.87	−16.6
	aug-cc-pVTZ[2]	−322.22	−1.9	−322.97	−2.7	−322.73	−2.4
	experimental[1]	−320.3		−320.3		−320.3	
8	aug-cc-pVDZ[2]	−438.17	7.4	−452.96	−7.4	−452.40	−6.8
	aug-cc-pVTZ[2]	−442.92	2.7	−447.42	−1.8	−446.81	−1.2
	experimental[1]	−445.6		−445.6		−445.6	
9	aug-cc-pVDZ[2]	−464.05	−17.4	−468.48	−21.8	−467.60	−20.9
	aug-cc-pVTZ[2]	−451.03	−4.3	−449.51	−2.8	−449.41	−2.7
	experimental[1]	−446.7		−446.7		−446.7	
10	aug-cc-pVDZ[2]	−526.86	17.3	−538.30	5.9	−538.68	5.5
	aug-cc-pVTZ[2]	−538.26	5.9	−542.02	2.2	−541.85	2.3
	experimental[1]	−544.2		−544.2		−544.2	
11	aug-cc-pVDZ[2]	−567.39	−2.5	−581.75	−16.9	−579.82	−14.9
	aug-cc-pVTZ[2]	−560.45	4.4	−566.83	−1.9	−565.78	−0.9
	experimental[1]	−564.9		−564.9		−564.9	
12	aug-cc-pVDZ[2]	−810.59	35.1	−829.80	15.9	−830.88	14.8
	aug-cc-pVTZ[2]	−832.42	13.3	−840.59	5.1	−840.36	5.3
	experimental[1]	−845.7		−845.7		−845.7	

[1] The valence correlation energy plus the Hartree-Fock energy computed in the given basis set plus core correlation energy from Table V in the main text.

[2] The difference between the computed reaction energy and the experimental value.

TABLE VI: The electronic reaction energies, $\Delta H_e^0(0\mathrm{K})$, (in kJ/mol) for the 12 test reactions[1].

		CCSD(T)		$\mathrm{CCSD(T)}_{\overline{\mathrm{R12}}}$			
				d			
		E	$\Delta_{\mathrm{experimental}}$ [2]	E	$\Delta_{\mathrm{experimental}}$ [2]	E	$\Delta_{\mathrm{experimental}}$ [2]
1	aug-cc-pVDZ[2]	−10.54	11.3	−19.09	2.7	−19.80	2.0
	aug-cc-pVTZ[2]	−20.90	0.9	−22.64	−0.8	−22.54	−0.7
	experimental[1]	−21.8		−21.8		−21.8	
2	aug-cc-pVDZ[2]	−145.49	19.9	−162.18	3.2	−162.54	2.9
	aug-cc-pVTZ[2]	−162.98	2.4	−166.16	−0.8	−165.67	−0.3
	experimental[1]	−165.4		−165.4		−165.4	
3	aug-cc-pVDZ[2]	−207.74	−3.8	−208.50	−4.6	−207.94	−4.0
	aug-cc-pVTZ[2]	−206.50	−2.6	−205.62	−1.7	−205.63	−1.7
	experimental[1]	−203.9		−203.9		−203.9	
4	aug-cc-pVDZ[2]	−228.79	16.5	−244.06	1.2	−244.55	0.8
	aug-cc-pVTZ[2]	−245.77	−0.5	−245.46	−0.2	−244.93	0.4
	experimental[1]	−245.3		−245.3		−245.3	
5	aug-cc-pVDZ[2]	−240.15	11.7	−249.29	2.6	−249.65	2.3
	aug-cc-pVTZ[2]	−250.01	1.9	−250.82	1.1	−250.56	1.3
	experimental[1]	−251.9		−251.9		−251.9	
6	aug-cc-pVDZ[2]	−250.69	23.1	−268.38	5.4	−269.45	4.4
	aug-cc-pVTZ[2]	−270.91	2.9	−273.46	0.3	−273.10	0.7
	experimental[1]	−273.8		−273.8		−273.8	
7	aug-cc-pVDZ[2]	−308.36	11.9	−321.32	−1.0	−321.65	−1.4
	aug-cc-pVTZ[2]	−320.97	−0.7	−321.73	−1.4	−321.48	−1.2
	experimental[1]	−320.3		−320.3		−320.3	
8	aug-cc-pVDZ[2]	−430.17	15.4	−444.97	0.6	−444.41	1.2
	aug-cc-pVTZ[2]	−442.35	3.2	−446.85	−1.3	−446.24	−0.6
	experimental[1]	−445.6		−445.6		−445.6	
9	aug-cc-pVDZ[2]	−446.45	0.2	−450.88	−4.2	−450.00	−3.3
	aug-cc-pVTZ[2]	−449.85	−3.2	−448.33	−1.6	−448.23	−1.5
	experimental[1]	−446.7		−446.7		−446.7	
10	aug-cc-pVDZ[2]	−529.56	14.6	−541.00	3.2	−541.38	2.8
	aug-cc-pVTZ[2]	−538.73	5.5	−542.49	1.7	−542.32	1.9
	experimental[1]	−544.2		−544.2		−544.2	
11	aug-cc-pVDZ[2]	−554.64	10.3	−569.01	−4.1	−567.07	−2.2
	aug-cc-pVTZ[2]	−560.83	4.1	−567.21	−2.3	−566.16	−1.3
	experimental[1]	−564.9		−564.9		−564.9	
12	aug-cc-pVDZ[2]	−820.40	25.3	−839.61	6.1	−840.69	5.0
	aug-cc-pVTZ[2]	−834.11	11.6	−842.27	3.4	−842.04	3.7
	experimental[1]	−845.7		−845.7		−845.7	

[1] T. Helgaker, P. Jørgensen, and J. Olsen, *Modern Electronic Structure Theory* (Wiley, Chichester, 2000), 1st ed.
[2] D. W. Schwenke, J. Chem. Phys. **122**, 014107 (2005).

[1] The valence correlation energy in the given basis plus the CBS Hartree Fock energy plus the core-correlation energy, both found in Table V in the main text.
[2] The difference between the computed reaction energy and the corresponding experimental value.