Supplementary Materials: Group Contribution Revisited: The Enthalpy of Formation of Organic Compounds with "Chemical Accuracy" Part II

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Table S1. Experimental and model values for mono-methylalkanes, where for the model values for the 2-methylalkanes a correction of −2.1 kJ/mol has been added to account for the geminal effect (see text). All values in kJ/mol. When available, Rossini c.s. data [18] were used when comparing with the present model (model – exp), otherwise NIST data, and when both were not available CAPEC data [12]. The red value 1.08 kJ/mol in the last row is the averaged absolute difference between the model Equation (4) and the experimental values. It may be recalled that the CH_2 increment for 2-methylnonane (−22.35 kJ/mol) is an indicator for an error in the experimental value (−260.2 kJ/mol) [1] which might explain the larger deviation though still within chemical accuracy.

Monomethyl alkanes	Rossini	NIST	NIST incr.	model dH	model-exp + correction (−2.1)	ABS (model-exp)
2-methylpropane	−131.7	−134.9		−131.08	−1.48	1.48
2-methylbutane	−154.6	−154.1	−19.20	−151.71	0.79	0.79
2-methylpentane	−174.43	−174.3	−20.20	−172.34	−0.01	0.01
2-methylhexane	−195.1	−195.5	−21.20	−192.97	0.03	0.03
2-methylheptane	−215.63	−215.5	−20.00	−213.6	−0.07	0.07
2-methyloctane				−234.23	−0.43	0.43
2-methylnonane		−260.2	−22.35	−254.86	3.24	3.24
3-methylpentane	−171.8	−171.6		−172.34	−0.54	0.54
3-methylhexane	−192.4	−192.5	−20.90	−192.97	−0.57	0.57
3-methylheptane	−212.78	−212.6	−20.10	−213.6	−0.82	0.82
4-methylheptane	−212.24	−212.1		−213.6	−1.36	1.36
4-methyloctane				−234.23	0.97	0.97
5-methylnonane		−258.6	−23.25	−254.86	3.74	3.74
averaged absolute difference						1.08

Table S2. Experimental and model values for dimethylalkanes. All values in kJ/mol. When available, Rossini c.s. data [18] available CAPEC data (not shown). The red value 1.08 kJ/mol in the last row is the averaged absolute difference between the final model (for discussion see text) and the experimental values.

Dimethyl alkanes	Rossini	NIST	model dHf	model-exp	ABS (model-exp)	model-exp + correction	ABS (model-exp+corr.)
2,2-dimethylpropane	−166.10	−168	−170.44	−4.34	4.34	−1.74	1.74
2,2-dimethylbutane	−185.70	−185.6	−191.07	−5.37	5.37	1.43	1.43
2,2-dimethylpentane	−206.38	−208	−211.7	−5.32	5.32	1.48	1.48
2,2-dimethylhexane	−224.88	−224.7	−232.33	−7.45	7.45	−0.65	0.65
2,2-dimethylheptane		−246.1	−252.96	−6.86	6.86	−0.06	0.06
2,3-dimethylbutane	−177.90	−177.8	−177.44	0.46	0.46	0.06	0.06
2,3-dimethylpentane	−199.40	−199	−198.07	1.33	1.33	3.03	3.03
2,3-dimethylhexane	−214.10	−213.9	−218.7	−4.60	4.6	−2.90	2.9
3,4-dimethylhexane	−213.16	−213	−218.7	−5.54	5.54	−1.74	1.74
2,4-dimethylpentane	−202.20	−203.5	−198.07	4.13	4.13	−0.07	0.07
2,4-dimethylhexane	−219.60	−219.4	−218.7	0.90	0.9	−1.20	1.2
2,5-dimethylhexane	−222.80	−222.6	−218.7	4.10	4.1	−0.10	0.1
2,6-dimethylheptane			−239.33	3.47	3.47	−0.73	0.73
2,6-dimethyloctane			−259.96	1.14	1.14	−0.96	0.96
2,7-dimethyloctane			−259.96	4.04	4.04	−0.16	0.16
3,3-dimethylpentane	−201.70	−204	−211.7	−10.00	10	1.00	1
3,3-dimethylhexane	−220.28	−220.1	−232.33	−12.05	12.05	−1.05	1.05
averaged absolute difference					4.77		1.08

Table S3. Experimental and model values for trimethylalkanes. All values in kJ/mol. Experimental data from Rossini c.s. [19] were used to compe with the present model (model – exp). The red value 1.18 kJ/mol in the last row is the averaged absolute difference between the final model (for discussion see text) and the experimental values.

Trimethyl alkanes	Rossini	model dHf	model-exp	ABS (model-exp)	model-exp + correction	ABS (model-exp + correction)	ABS (model-exp + correction + Me-Me-1,5-interaction)
2,2,3-trimethylbutane	−205.00	−216.8	−11.80	11.8	−1.30	1.3	1.30
2,2,3-trimethylpentane	−220.30	−237.43	−17.13	17.13	−2.73	2.73	2.73
2,2,4-trimethylpentane	−224.30	−237.43	−13.13	13.13	−8.43	8.43	0.07
2,3,3-trimethylpentane	−216.60	−237.43	−20.83	20.83	−4.33	4.33	4.33
2,3,4-trimethylpentane	−217.60	−223.8	−6.20	6.2	−2.80	2.8	2.80
2,2,5-trimethylhexane	−254.19	−258.06	−3.87	3.87	0.83	0.83	0.83
2,4,4-trimethylhexane	−241.00	−258.06	−17.06	17.06	−8.16	8.16	0.34
2,3,3-trimethylhexane	−238.99	−258.06	−19.07	19.07	−2.57	2.57	2.57
2,2,3-trimethylhexane	−241.38	−258.06	−16.68	16.68	−2.28	2.28	2.28
2,2,4-trimethylhexane	−243.39	−258.06	−14.67	14.67	−7.87	7.87	0.63
2,3,4-trimethylhexane	−235.23	−244.43	−9.20	9.2	−3.70	3.7	3.70
2,3,5-trimethylhexane	−242.97	−244.43	−1.46	1.46	−1.86	1.86	1.86
3,3,4-trimethylhexane	−236.10	−258.06	−21.96	21.96	−3.36	3.36	3.36
averaged absolute difference				13.31		3.86	2.06

Table S4. Experimental and model values for tetramethylalkanes. All values in kJ/mol. Rossini c.s. data [19] except for 2,2,5,5-tetramethylhexane (CAPEC data base) were used when comparing with the present model (model – exp). The red value 3.27 kJ/mol in the last row is the averaged absolute difference between the final model (for discussion see text) and the experimental values.

Tetramethyl alkanes	Rossini	model dHf	model-exp	ABS (model-exp)	model-exp + correction	ABS(model-exp+ correction)	ABS (model-exp + correction + Me-Me-1,5-interaction)
2,2,3,3-tetramethylbutane	−226.06	−256.16	−30.10	30.1	−1.30	1.3	1.30
2,2,3,4-tetramethylpentane	−237.15	−263.16	−26.01	26.01	−9.91	9.91	1.41
2,2,3,3-tetramethylpentane	−237.40	−276.79	−39.39	39.39	−6.39	6.39	6.39
2,2,4,4-tetramethylpentane	−242.13	−276.79	−34.66	34.66	−21.06	21.06	4.06
2,3,3,4-tetramethylpentane	−236.40	−263.16	−26.76	26.76	−4.76	4.76	4.76
2,2,5,5-tetramethylhexane		−297.42	−11.92	11.92	1.68	1.68	1.68
averaged absolute difference				28.14		7.52	3.27

Table S5. Experimental and model values for pentamethylalkanes. All values in kJ/mol. When available, Experimental data from Rossini c.s. [19] were used when comparing with the present model (model – exp). Corrections as described in the text.

Pentamethyl alkanes	Rossini	model dHf	model-exp	ABS (model-exp)	model-exp + correction	ABS(model-exp + correction)	ABS (model-exp + correction + Me-Me-1,5-interaction)
2,2,3,3,4-pentamethylpentane	−247.4	−302.52	−55.12	55.12	−16.62	16.62	8.12
2,2,3,4,4-pentamethylpentane	−247.2	−302.52	−55.32	55.32	−26.52	26.52	9.52

Table S6. Experimental and model values for ethylalkanes. All values in kJ/mol. Experimental data were taken from Rossini c.s., i.e. the first two entries from Prosen and Rossini [18] and all others from Labbauf et al. [19]. Upper table: mono up to tri-substituted alkanes. The red value 1.62 kJ/mol in the last row is the averaged absolute difference between the final model (for discussion see text) and the experimental values. Lower table: tetra-substituted alkanes.

Ethyl and propyl alkanes	Rossini	model dHf	model-exp	ABS (model-exp)	model-exp + correction	model-exp + correction + corr.ethyl /propyl	ABS(model-exp+ correction + corr.ethyl)
3-ethylpentane	−189.80	−192.97	−3.17	3.17	−3.17	2.83	2.83
3-ethylhexane	−211	−213.6	−2.6	2.6	−2.60	3.40	3.4
3-ethylheptane	−230.6	−234.23	−3.63	3.63	−3.63	2.37	2.37
4-ethylheptane	−230.6	−234.23	−3.63	3.63	−3.63	2.37	2.37
3-ethyloctane	−251.3	−254.86	−3.56	3.56	−3.56	2.44	2.44
4-ethyloctane	−251.3	−254.86	−3.56	3.56	−3.56	2.44	2.44
3-methyl-3-ethylpentane	−215.1	−232.33	−17.23	17.23	−6.23	−0.23	0.23
2-methyl-3-ethylpentane	−211.36	−218.7	−7.34	7.34	−3.54	0.36	0.36
2-methyl-3-ethylhexane	−232.9	−239.33	−6.43	6.43	−2.63	1.27	1.27
2-methyl-4-ethylhexane	−237.8	−239.33	−1.53	1.53	−1.53	2.37	2.37
3-methyl-3-ethylhexane	−236.5	−252.96	−16.46	16.46	−5.46	0.54	0.54
3-methyl-4-ethylhexane	−230	−239.33	−9.33	9.33	−5.53	0.47	0.47
2-methyl-3-ethylheptane	−253.6	−259.96	−6.36	6.36	−4.66	1.34	1.34
2-methyl-4-ethylheptane	−258.4	−259.96	−1.56	1.56	−3.66	2.34	2.34
2-methyl-5-ethylheptane	−258.4	−259.96	−1.56	1.56	−3.66	2.34	2.34
3-methyl-3-ethylheptane	−257.1	−273.59	−16.49	16.49	−5.49	0.51	0.51
3-methyl-4-ethylheptane	−250.7	−259.96	−9.26	9.26	−5.46	0.54	0.54
3-methyl-5-ethylheptane	−255.6	−259.96	−4.36	4.36	−4.36	1.64	1.64
4-methyl-4-ethylheptane	−257.1	−273.59	−16.49	16.49	−5.49	0.51	0.51
2,2-dimethyl-3-ethylpentane	−238.5	−258.06	−19.56	19.56	−5.16	0.84	0.84
2,3-dimethyl-3-ethylpentane	−233.7	−258.06	−24.36	24.36	−7.86	−1.86	1.86
2,4-dimethyl-3-ethylpentane	−235.2	−244.43	−9.23	9.23	−5.83	0.17	0.17
3,3,-diethylpentane	−232.1	−252.96	−20.86	20.86	−9.86	2.14	2.14
3,3-diethylhexane	−251.85	−273.59	−21.74	21.74	−10.74	1.26	1.26
3,4-diethylhexane	−247.8	−259.96	−12.16	12.16	−8.36	3.64	3.64
4-n-propylheptane	−251.3	−254.86	−3.56	3.56	−3.56	2.44	2.44
4-isopropylheptane	−253.6	−259.96	−6.36	6.36	−6.36	−0.36	0.36
2-methyl-3-isopropylhexane	−255.9	−265.06	−9.16	9.16	−7.46	−1.46	1.46
2,3-dimethyl-3-isopropylpentane	−258.2	−283.79	−25.59	25.59	−9.09	−3.09	3.09
2-methyl-3,3-diethylpentane	−249.1	−278.69	−29.59	29.59	−13.09	−1.09	1.09
averaged absolute difference				10.56			1.62

	Rossini	model dHf	model-exp	ABS(model-exp)	model-exp + correction	model-exp + correction + corr.ethyl /propyl	ABS(model-exp+ correction + corr.ethy + Me-Me-1,5-interaction)
2,2,3-trimethyl-3-ethylpentane	−252.8	−297.42	−44.62	44.62	−9.46	−3.46	3.46
2,2,4-trimethyl-3-ethylpentane	−253.5	−283.79	−30.29	30.29	−10.39	−4.39	4.11
2,3,4-trimethyl-3-ethylpentane	−251.6	−283.79	−32.19	32.19	−10.19	−4.19	4.31
3,3,4,4-tetraethylhexane	−264.3	−379.94	−115.64	115.64	−78.44	−54.44	54.44

Table S7. Experimental and model values for various alcohols. All values in kJ/mol. Experimental data were taken from Verevkin [21]. The red values are averaged absolute differences between the final model (for discussion see text) and the experimental values.

Alcohols	Verevkin [2005]	model dHf	model-exp	ABS (model-exp)	
ethanol	−234	−233.99	0.01	0.01	
1-propanol	−256	−254.62	1.38	1.38	
1-butanol	−274.9	−275.25	−0.35	0.35	
2-butanol	−293.01	−292.85	0.16	0.16	
1-pentanol	−294.7	−295.88	−1.18	1.18	
2-pentanol	−311	−313.48	−2.48	2.48	
3-pentanol	−316	−313.48	2.52	2.52	
1-hexanol	−315.8	−316.51	−0.71	0.71	
2-hexanol	−335	−334.11	0.89	0.89	
3-hexanol	−331.7	−334.11	−2.41	2.41	
1-heptanol	−336.5	−337.14	−0.64	0.64	
2-heptanol	−354.8	−354.74	0.06	0.06	
3-heptanol	−357.8	−354.74	3.06	3.06	
4-heptanol	−353.9	−354.74	−0.84	0.84	
1-octanol	−356.5	−357.77	−1.27	1.27	
2-octanol	−373.6	−375.37	−1.77	1.77	
3-octanol	−375.4	−375.37	0.03	0.03	
4-octanol	−368.8	−375.37	−6.57	6.57	
1-nonanol	−378.9	−378.4	0.50	0.5	
1-decanol	−397.2	−399.03	−1.83	1.83	
1-undecanol	−420.2	−419.66	0.54	0.54	
1-dodecanol	−438.5	−440.29	−1.79	1.79	
1-tetradecanol	−482.7	−481.55	1.15	1.15	
averaged absolute difference				1.40	
2-methyl-1-butanol	−302.5	−300.98	1.52	1.52	
3-methyl-1-butanol	−301.6	−300.98	0.62	0.62	
2-methyl-2-butanol	−331.8	−332.21	−0.41	0.41	
3-methyl-2-butanol	−318.3	−318.58	−0.28	0.28	
2,3-dimethyl-2-butanol	−357	−357.94	−0.94	0.94	
2-methyl-2-pentanol	−353.8	−352.84	0.96	0.96	
4-methyl-2-pentanol	−337.4	−339.21	−1.81	1.81	
2-methyl-3-pentanol	−340.4	−339.21	1.19	1.19	
3-methyl-3-pentanol	−350.6	−352.84	−2.24	2.24	
2-methyl-2-hexanol	−376.6	−373.47	3.13	3.13	
2-ethyl-1-hexanol	−364.8	−362.87	1.93	1.93	
averaged absolute difference				1.37	
					ABS (model-exp + correction + Me-Me-1,5-interaction)
3,5,5-trimethyl-1-hexanol	−389	−399.53	−10.53	10.53	2.03
2,2,4,4-tetramethyl-3-pentanol	−397	−443.66	−17.86	17.86	0.86
2,2,4,4-tetramethyl-3-iPr-3-pentanol	−418.1	−529.38	−50.28	50.28	33.28