TEMPERATURE DEPENDENCE OF THERMOCHEMICAL QUANTITIES. PARAMETERS OF THE POLYNOMIAL $C^0_{p,T}=a+bT+cT^2+dT^3$ FROM GROUP CONTRIBUTIONS

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Group contributions to the parameters of the polynomial

$$C^0_{p,T} = a+bT+cT^2+dT^3$$

have been calculated. This procedure extends the scope of application of the C^0_p function in the above form for the fast and precise calculation of the temperature-dependence of various thermochemical quantities.

Molar heat capacities (C^0_p) of different species have been described in the polynomial form:

$$C^0_{p,T} = a+bT+cT^2+dT^3 \tag{1}$$

in a previous paper [1]. Such a procedure makes the calculation of the temperature-dependence of various thermochemical and kinetic quantities simple. Usage of a computer program (see *e.g.* the program KIRCH in [2]) makes the calculations less tiresome, although they can also be performed with a pocket calculator. The data collected in [1] permit calculations only in cases when the data required are available for all the species involved.

It has been shown that our knowledge can be widened considerably by using group values to estimate the missing thermochemical data (see *e.g.* BENSON [3]). However, to use C^0_p expressed by equation (1) in the calculation of thermochemical data at higher temperatures, a computer program must be available to perform the non-linear least squares calculations. This circumstance may cause some difficulty in the application of the suggested procedure.

To overcome this difficulty, the parameters of equation (1) have been calculated from BENSON's group values [3]. The parameters of the C^0_p functions of many species can now be obtained by summing the contributions of the various groups:

$$C^0_p = \sum_i a_i + T \sum_i b_i + T^2 \sum_i c_i + T^3 \sum_i d_i \tag{2}$$

where subscript i refers to the i-th group of the species concerned. Thus, the scope of application of the C^0_p function in the polynomial form for the calculation of various thermochemical quantities [1] can be extended considerably.

Table I

Thermochemical data of various species in the gas phase Hydrocarbon groups

No.	Group		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	a·10/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	b·10^2/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	c·10^6/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	d·10^9/ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
1	$[C-(H)_3(C)]$	C	−10.20	30.41	−0.12857	2.35477	−10.1393	1.37028
		J	−42.68	127.24	−0.53794	9.85236	−42.4228	5.73325
2	$[C-(H)_2(C)_2]$	C	−4.93	9.42	−3.24681	2.32747	−13.9412	3.32925
		J	−20.63	39.41	−13.5847	9.73813	−58.3300	13.9296
3	$[C-(H)(C)_3]$	C	−1.90	−12.07	−20.2397	2.82589	−23.3852	7.21075
		J	−7.95	−50.50	−84.6831	11.8235	−97.8437	30.1697
4	$[C-(C)_4]$	C	0.50	−35.10	−50.1623	4.34818	−45.2765	15.5862
		J	2.09	−146.86	−209.879	18.1928	−189.437	65.2127
5	$[C_d-(H)_2]$	C	6.26	27.61	1.34016	1.95726	−10.8810	2.44350
		J	26.19	115.52	5.60723	8.18917	−45.5261	10.2236
6	$[C_d-(H)(C)]$	C	8.59	7.97	10.6499	1.15718	−4.15577	−0.03039
		J	35.94	33.35	44.5592	4.48164	−17.3877	−0.12715
7	$[C_d-(C)_2]$	C	10.34	−12.70	21.4700	0.81169	−5.64587	1.46702
		J	43.23	−53.14	89.8305	3.39611	−23.6223	6.13801
8	$[C_d-(C_d)(H)]$	C	6.78	6.38	−21.3988	3.01542	−30.5372	11.5164
		J	28.37	26.69	−89.5325	12.6156	−127.768	48.1846
9	$[C_d-(C_d)(C)]$	C	8.88	−14.6	−10.5741	2.66979	−32.0174	13.0129
		J	37.15	−61.09	−44.2421	11.1704	−133.961	54.4460
10	$[C_d-(C_B)(H)]$	C	6.78	6.38	−21.3913	3.01520	−30.5237	11.5153
		J	28.37	26.69	−89.5014	12.6165	−127.711	48.1800
11	$[C_d-(C_B)(C)]$	C	8.64	−14.6	−10.5741	2.66979	−32.0174	13.0129
		J	36.15	−61.09	−44.2421	11.1702	−133.961	54.4460
12	$[C_d-(C_t)(H)]$	C	6.78	6.38	−21.3913	3.0152	−30.5237	11.5153
		J	28.37	26.69	−89.5012	12.6156	−127.711	48.1800
13	$[C_d-(C_B)_2]$	C	8.0					
		J	33.47					
14	$[C_d-(C_d)_2]$	C	4.6					
		J	19.25					
15	$[C-(C_d)(C)(H)_2]$	C	−4.76	9.80	−25.4663	3.24954	−25.6242	8.16307
		J	−19.92	41.00	−106.551	13.5960	−107.212	34.1543
16	$[C-(C_d)_2(H)_2]$	C	−4.29	10.2	−54.1897	4.53600	−43.5877	16.2486
		J	−17.95	42.68	−226.730	18.9786	−182.371	67.9841
17	$[C-(C_d)(C_B)(H)_2]$	C	−4.29	10.2	−54.1897	4.5360	−43.5877	16.2485
		J	−17.95	42.68	−226.730	18.9786	−182.371	67.9841
18	$[C-(C_t)(C)(H)_2$	C	−4.73	10.30	−17.4220	2.75939	−19.3447	5.68257
		J	−19.79	43.09	−72.8936	11.5453	−80.9382	23.7759

19	$[C-(C_B)(C)(H)_2]$	C	−4.86	9.34	−24.7360	3.67869	−33.8089	12.0376
		J	−20.33	39.08	−103.495	15.3916	−141.456	50.3653
20	$[C-(C_d)(C)_2(H)]$	C	−1.48	−11.69	−46.8767	3.99092	−38.9247	13.8966
		J	−6.19	−48.91	−196.132	16.6980	−162.861	58.1434
21	$[C-(C_t)(C)_2(H)]$	C	−1.72	−11.19	−34.4194	3.25794	−28.7990	9.56459
		J	−7.20	−46.82	−144.011	13.6312	−120.495	40.0182
22	$[C-(C_B)(C)_2(H)]$	C	−0.98	−12.15	−42.5272	4.21317	−43.6737	16.0478
		J	−4.10	−50.83	−177.934	17.6279	−182.731	67.1440
23	$[C-(C_d)(C)_3]$	C	1.68	−34.72	−73.4441	5.33751	−58.3124	21.2436
		J	7.03	−145.27	−307.290	22.3321	−243.979	88.8832
24	$[C-(C_B)(C)_3]$	C	2.81	−35.18	−93.2429	6.68319	−79.3496	30.8155
		J	11.75	−147.19	−390.128	27.9625	−331.999	128.932
25	$[C_t-(H)]$	C	26.93	24.7	18.7311	1.5457	−15.5117	6.14453
		J	112.67	103.34	78.3708	6.46729	−64.9010	25.7087
26	$[C_t-(C)]$	C	27.55	6.35	20.1401	0.38202	0.05672	−0.85646
		J	115.27	26.57	84.2664	1.59837	0.23732	−3.58343
27	$[C_t-(C_d)]$	C	29.20	6.43	9.34644	0.37397	8.49730	−7.68715
		J	122.17	26.90	39.1055	1.56469	35.5527	−32.1630
28	$[C_t-(C_B)]$	C	29.20	6.43	9.34644	0.37397	8.49730	−7.68715
		J	122.17	26.90	39.1055	1.56469	35.5527	−32.1630
29	$[C_B-(H)]$	C	3.30	11.53	−18.6837	2.12158	−15.3099	4.37156
		J	13.80	48.24	−78.1728	8.87669	−64.0566	18.2906
30	$[C_B-(C)]$	C	5.51	−7.69	14.0046	0.31667	4.57456	−3.70304
		J	23.05	−32.1750	58.5952	1.32490	19.1400	−15.4935
31	$[C_B-(C_d)]$	C	5.68	−7.80	23.4057	0.40374	0.84074	−1.60942
		J	23.76	−32.64	97.9294	1.68925	3.51766	−6.73381
32	$[C_B-(C_t)]$	C	5.68	−7.80	23.4056	0.40374	0.84038	−1.60942
		J	23.76	−32.64	97.9294	1.68925	3.51615	−6.73386
33	$[C_B-(C_B)]$	C	4.96	−8.64	−13.2698	2 14419	−22.0807	7.91812
		J	20.75	−36.15	−55.5210	8.9713	−92.3856	33.1294
34	$[C_a]$	C	34.20	6.0	15.6166	1.05932	−10.3753	3.72057
		J	143.09	25.10	65.3399	4.43220	−43.4103	15.5669
35	$[C_{BF}-(C_B)_2(C_{BF})]$	C	4.8	−5.0	0.72194	1.25303	−9.96682	2.86776
		J	20.08	−20.92	3.02059	5.24267	−41.7012	11.9987
36	$[C_{BF}-(C_B)(C_{BF})_2]$	C	3.7	−5.0	0.72194	1.25303	−9.96682	2.86776
		J	15.48	−20.92	3.02059	5.24267	−41.7012	11.9987
37	$[C_{BF}-(C_{BF})_3]$	C	1.5	1.4	−19.4352	1.73958	−15.5515	5.20323
		J	6.28	5.86	−81.3170	7.27840	−65.0675	21.7703
38	cis-Correction	C	1.00	0.0	−26.4775	0.54328	−4.02093	0.97260
		J	4.18	0.0	−110.781	2.27308	−16.8236	4.06936
39	ortho-Correction	C	0.57	−1.61	−8.18322	1.11744	−17.9844	8.29380
		J	2.38	−6.74	−34.2386	4.67539	−75.2467	34.7013

Corrections to be Applied to Ring-compound Estimates

Ring		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$a\cdot 10$/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$b\cdot 10^2$/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	$c\cdot 10^6$/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	$d\cdot 10^9$/ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
c-propane	C	27.6	32.1	−65.3780	1.69580	−20.4667	8.42331
	J	115.48	134.306	−273.541	7.09523	−85.6327	35.2431
c-butane	C	26.2	29.8	−79.7807	1.39105	−9.94155	2.62575
	J	109.62	124.68	−333.803	5.82015	−41.5957	10.9861
c-butene	C	29.8	29.0	−44.2188	0.85618	−8.54718	3.07453
	J	124.68	121.34	−185.012	3.58226	−35.7614	12.8638
c-pentane	C	6.3	27.3	−115.538	2.18462	−19.0291	6.80004
	J	26.36	114.22	−483.411	9.14045	−79.6178	28.4514
c-pentene	C	5.9	25.8	−63.4951	−0.27455	16.4327	−9.59419
	J	24.68	107.95	−265.663	−1.14872	68.7544	−40.1421
c-hexane	C	0.0	18.8	−91.8337	0.72720	18.1873	−14.0674
	J	0.0	78.66	−384.232	3.04260	76.0957	−58.8580
c-hexene	C	1.4	21.5	−96.5478	2.28373	−17.5803	4.48817
	J	5.86	89.96	−403.956	9.55513	−73.5560	18.77850

Oxygen-containing Compounds

No.	Group		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$a\cdot 10$/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$b\cdot 10^2$ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	$c\cdot 10^6$ cal mol^{-1}K^{-3} or J mol^{-} K^{-3}	$d\cdot 10^9$ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
1	[O(H)$_2$]	C	−57.8	45.1	95.3019	1.53611	41.4284	−24.5283
		J	−241.83	188.70	398.743	−6.42728	173.336	−102.626
2	[O(H)(C)]	C	−37.9	29.07	50.5235	−0.68993	16.9306	−8.48907
		J	−158.57	121.63	211.390	−2.88667	70.8376	−35.5183
3	[O(H)(C$_B$)]	C	−37.9	29.1	−197.615	10.6686	−147.479	67.2458
		J	−158.57	121.75	−826.821	44.6374	−617.052	281.356
4	[O(H)(O)]	C	−16.3	27.85	24.5178	1.17223	−9.41261	2.73694
		J	−68.20	116.52	102.582	4.90461	−39.3824	11.4514

5	[O(H)(CO)]	C	−58.1	24.5	−19.5360	2.66069	−27.7324	10.8889
		J	−243.09	102.51	−81.7388	11.1323	−116.032	45.5592
6	$[O(C)_2]$	C	−23.2	8.68	37.3508	−0.27931	7.37222	−3.69635
		J	−97.07	36.32	156.276	−1.16863	30.8454	−15.4655
7	[O(C)(O)]	C	−4.5	9.4	54.7563	−1.04219	18.0923	−8.93282
		J	−18.83	39.33	229.100	−4.36052	75.6982	−37.3749
8	$[O(O)_2]$	C	19.0	9.4	54.7563	−1.04219	18.0923	−8.93282
		J	79.50	39.33	229.100	−4.36052	75.6982	−37.3749
9	$[CO(H)_2]$	C	−26.0	52.3	32.4434	0.79426	42.8569	−39.1509
		J	−108.78	218.82	135.743	3.32319	179.313	−163.807
10	[CO(H)(C)]	C	−29.1	34.9	48.7824	0.47118	9.72417	−7.12061
		J	−121.75	146.02	204.105	1.97142	40.6859	−29.7926
11	[CO(H)(O)]	C	−32.1	34.9	46.2752	0.63639	6.79527	−5.58808
		J	−134.31	146.02	193.615	2.66266	28.4314	−23.3805
12	$[CO(C)_2]$	C	−31.4	15.0	33.6942	0.67153	3.34527	−3.83476
		J	−131.38	62.76	140.976	2.80968	13.9966	−16.0446
13	[CO(C)(O)]	C	−35.1	14.8	39.7537	0.61812	3.00834	−3.76826
		J	−146.86	61.92	166.330	2.58621	12.5869	−15.7664
14	$[C(H)_3(O)]$	C	−10.08	30.41	0.40061	2.32282	−9.55691	1.05477
		J	−41.27	127.24	1.67615	9.71868	−39.9861	4.41316
15	$[C(H)_2(O)(C)]$	C	−8.1	9.8	−34.6110	3.69163	−32.4810	11.3583
		J	−33.89	41.00	−144.812	15.4458	−135.901	47.5231
16	$[C(H)(O)(C)_2]$	C	−7.2	−11.0	−53.8976	4.78986	−52.5418	20.4416
		J	−30.12	−46.02	−225.508	20.0408	−219.835	85.5277
17	$[C(O)(C)_3]$	C	−6.6	−33.56	−62.1486	5.16292	−61.9195	24.7600
		J	−27.61	−140.415	−260.030	21.6017	−259.071	103.596
18	$[C(H)_3(CO)]$	C	−10.08	30.41	−0.12863	2.35477	−10.1394	1.37028
		J	−42.17	127.24	−0.53819	9.85236	−42.4232	5.73325
19	$[C(H)_2(CO)(C)]$	C	−5.2	9.6	3.59622	2.51711	−20.6641	7.34899
		J	−21.76	40.17	15.0466	10.5316	−86.4586	30.74817
20	$[C_d(O)(H)]$	C	8.6	8.0	46.2607	1.00718	89.6967	0.84507
		J	35.98	33.47	193.554	4.21404	375.291	3.53577
21	$[C_B(O)]$	C	−0.9	−10.2	−44.4976	4.06574	−48.3860	19.0831
		J	−3.77	−42.68	−186.178	17.0110	−202.447	79.8437
22		C	26.9	30.50	45.3787	−3.66015	57.1061	−27.3231
		J	112.55	127.61	189.865	−15.3141	238.932	−114.320
23		C	25.7	27.7	−53.1523	0.24028	−4.32367	7.38501
		J	107.53	115.90	−222.389	1.00533	−18.0902	30.8989

Nitrogen-containing Compounds

No.	Group		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$a \cdot 10$/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$b \cdot 10^2$/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	$c \cdot 10^6$/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	$d \cdot 10^9$ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
1	[C(N)(H)$_3$]	C	−10.08	30.41	−0.12858	2.35477	−10.1393	1.37029
		J	−42.17	127.24	−0.53798	9.85223	−42.4228	5.73329
2	[C—(N)(C)(H)$_2$]	C	−6.6	9.8	−18.9138	3.01262	−23.2942	7.40836
		J	−27.61	41.00	−79.1355	12.6048	−97.4629	30.9966
3	[C—(N)(C)$_2$(H)]	C	−5.2	−11.7	−37.3690	3.82532	−38.2549	13.9859
		J	−21.75	−48.95	−156.352	16.0051	−160.059	58.5170
4	[C—(N)(C)$_3$]	C	−3.2	−34.1	−56.1025	4.57138	−53.4861	20.1061
		J	−13.39	−142.67	−234.733	19.8798	−223.786	84.1239
5	[N—(C)(H)$_2$]	C	4.8	29.71	32.8362	0.78470	1.50372	−2.16489
		J	20.08	124.31	137.387	3.28318	6.29156	−9.05790
6	[N—(C)$_2$(H)]	C	15.4	8.94	−2.22472	1.83506	−13.2690	3.79109
		J	64.43	37.41	−9.30823	7.67789	−55.5175	15.8619
7	[N—(C)$_3$]	C	24.4	−13.46	−20.1529	2.45457	−22.9560	7.10337
		J	102.09	−56.32	−84.3198	10.2699	−96.0479	29.7205
8	[N—(N)(H)$_2$]	C	11.4	29.13	3.93839	2.44982	−20.3582	6.99005
		J	47.70	121.88	16.4782	10.2500	−85.1787	29.2464
9	[N—(N)(C)(H)]	C	20.9	9.61	3.45879	1.99764	−18.7173	6.70370
		J	87.45	40.21	14.4716	8.35813	−78.3132	28.0483
10	[N$_A$—(H)]	C	25.1	26.8	26.9021	0.55638	0.53168	−1.36833
		J	105.02	112.13	112.558	2.32789	2.22455	−5.72509
11	[N—(C$_B$)(H)$_2$]	C	4.8	29.71	32.8361	0.78470	1.50306	−2.16491
		J	20.08	124.31	137.386	3.28318	6.28880	−9.05798
12	[C$_B$—(N)]	C	−0.5	−9.69	−35.7156	3.69462	−44.8670	18.0561
		J	−2.09	−40.54	−149.434	15.4583	−187.724	75.5467
13	[CO—(N)(H)]	C	−29.6	34.93	46.3301	0.65844	6.03398	−5.05496
		J	−123.85	146.147	193.845	2.75491	25.2462	−21.1500
14	[CO—(N)(C)]	C	−32.8	16.2	36.8768	0.38941	7.00140	−3.37865
		J	−137.24	67.78	154.292	1.62929	29.2939	−14.1363
15	[N—(CO)(H)$_2$]	C	−14.9	24.69	−32.5291	3.09738	−24.2736	7.77065
		J	−62.34	103.30	−136.102	12.9594	−101.561	32.5124
16	[C—(CN)(C)(H)$_2$]	C	22.5	40.20	15.9367	3.80737	−22.8625	4.49026
		J	94.14	168.20	66.6793	15.9300	−95.6567	18.7872
17	[C—(CN)(C)$_2$(H)]	C	25.8	19.80	44.5475	2.59553	−14.5810	2.77019
		J	107.95	82.84	186.387	10.8597	−61.0069	11.5905
18	[C$_d$—(CN)(H)]	C	37.4	36.58	16.2789	3.41575	−25.0051	6.52183
		J	156.48	153.05	68.1111	14.2915	−104.621	27.2873

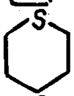
19	[C_d—(NO_2)(H)]	C	0.0	44.4	−6.46303	5.59142	−47.2394	15.1674
		J	0.0	185.77	−27.0413	23.3945	−197.648	63.4604
20	[C_B(CN)]	C	35.8	20.50	31.3116	2.94963	−27.0020	9.27539
		J	149.79	85.77	131.008	12.3413	−112.976	38.8082
21	[C_t—(CN)]	C	63.8	35.4	55.9837	2.07473	−19.0015	6.95655
		J	266.94	148.11	234.236	8.68067	−79.5002	29.1062
22	[O—(NO)(C)]	C	−5.9	41.9	49.5292	1.59512	−6.72626	−0.27066
		J	−24.69	175.31	207.230	6.67398	−28.1427	−1.13244
23	[C—N_A)$(H)_3$]	C	−10.08	30.41	−0.12858	2.35477	−10.1392	1.37028
		J	−42.17	127.23	−0.53798	9.85223	−42.4224	5.73329
24	[C—(N_A)(C)$(H)_2$]	C	−5.50	9.42	−3.24681	2.32747	−13.9382	3.32919
		J	−23.01	39.41	−13.5846	9.73813	−58.3174	13.9293
25	[C—(N_A)$(C)_2$(H)]	C	−3.30	−12.07	−20.2397	2.82589	−23.3852	7.21075
		J	−13.81	−50.50	−84.6829	11.8235	−97.8437	30.1698
26	[C—N_A)$(C)_3$]	C	−1.90	−35.10	−50.1623	4.34818	−45.2765	15.5862
		J	−7.95	−146.86	−209.879	18.1928	−189.437	65.2118
27	[N_A—(C)]	C	32.50	8.0	18.8316	1.00732	−11.3817	4.73510
		J	135.98	33.47	78.7914	2.21463	−47.6210	19.8117

Halogen-containing Compounds

1	[C—$(F)_3$(C)]	C	−158.4	42.5	25.2890	4.46920	−39.2869	12.0644
		J	−662.75	177.82	105.809	18.6991	−164.376	50.4774
2	[C—(F)$(H)_2$(C)]	C	−51.5	35.4	−7.97369	3.75980	−29.5153	9.32093
		J	−215.48	148.11	−33.3619	15.7310	−123.492	38.9988
3	[C—$(Cl)_3$(C)]	C	−20.7	50.4	73.2732	4.22792	−46.3482	17.7478
		J	−86.61	210.87	306.575	17.6896	−193.920	74.2568
4	[C—$(Cl)_2$(H)(C)]	C	−18.9	43.7	32.6693	3.89784	−35.1709	11.6275
		J	−79.08	182.84	136.688	16.3086	−147.155	48.6495
5	[C—(Cl)$(H)_2$(C)]	C	−16.5	37.8	7.64606	3.48116	−28.6314	9.75781
		J	−69.04	158.16	31.9911	14.5652	−119.794	40.8267
6	[C—$(Br)_3$(C)]	C		55.7	94.9607	3.44283	−39.3741	15.7495
		J		233.05	397.316	14.4048	−164.741	65.8959
7	[C—(Br)$(H)_2$(C)]	C	−5.4	40.8	2.48882	3.86772	−34.2162	12.0933
		J	−22.59	170.71	10.4132	16.1825	−143.161	50.5984
8	[C—(I)$(H)_2$(C)]	C	8.0	43.0	0.55952	3.97186	−34.9545	12.3784
		J	33.47	179.91	2.34103	16.6183	−146.250	51.7912
9	[C—(I)(H)$(C)_2$]	C	10.5	21.3	8.88289	3.74583	−36.1824	12.6422
		J	43.93	89.12	37.1660	15.6726	−151.387	52.8950
10	[C—(Cl)(Br)(H)(C)]	C		45.70	41.6428	3.66912	−34.8906	13.0415
		J		191.21	174.234	15.3516	−145.982	54.5656

No.	Group		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	a·10/ cal mol^{-1}K^{-1} or J mol^{-1} K^{-1}	b·10^3/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	c·10^6/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	d·10^9/ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
11	[C_d—(F)$_2$]	C	−77.5	37.3	36.9318	2.65499	−24.1777	8.43921
		J	−324.26	156.06	154.523	11.1085	−101.159	35.3097
12	[C_d—(Cl)$_2$]	C	−1.8	42.1	59.7574	2.44749	−23.7920	8.34164
		J	−7.53	176.15	250.025	10.2403	−99.5457	34.9014
13	[C_d—(Br)$_2$]	C		47.6	77.3479	2.07955	−20.7993	7.47221
		J		199.16	323.624	8.70083	−87.0243	31.2637
14	[C_d—(F)(Cl)]	C		39.8	36.8044	3.01484	−29.9309	10.8079
		J		166.52	153.990	12.6141	−125.231	45.2203
15	[C_d—(F)(Br)]	C		42.5	53.5284	2.40967	−21.7542	7.00641
		J		177.82	223.963	10.0821	−91.0196	29.3148
16	[C_d—(Cl)(Br)]	C		45.1	96.9061	0.76529	2.27788	−4.93257
		J		188.7	405.455	3.20197	9.53065	−20.6379
17	[C_d—(F)(H)]	C	−37.6	32.8	−2.62884	3.09623	−27.3390	9.34189
		J	−157.32	137.24	−10.991	12.9546	−114.386	39.0865
18	[C_d—(Cl)(H)]	C	−1.2	35.4	17.4843	2.65290	−22.4436	7.26045
		J	−5.02	148.11	73.1543	11.0997	−93.9040	30.3777
19	[C_d—(Br)(H)]	C	11.0	38.3	9.01923	3.26919	−32.8267	12.4304
		J	46.02	160.25	37.7365	13.6783	−137.347	52.0088
20	[C_d—(I)(H)]	C	24.5	40.5	32.5676	2.45017	−22.3799	7.92354
		J	102.51	169.45	136.263	10.2515	−93.6375	33.1521
21	[C_t—(Cl)]	C		33.4	59.1678	0.85088	−6.75683	1.93400
		J		139.75	247.560	3.56008	−28.2706	8.09186
22	[C_t—(Br)]	C		36.1	63.3969	0.88870	−8.79468	3.26923
		J		151.04	265.253	3.71832	−36.7969	13.6785
23	[C_t—(I)]	C		37.9	64.3969	0.88870	−8.79468	3.26923
		J		158.57	269.437	3.71832	−36.7969	13.6785
24	[C_B—(F)]	C	−42.8	16.1	−4.77662	3.14999	−33.3810	12.5612
		J	−179.08	67.36	−19.9854	13.1796	−139.666	52.5561
25	[C_B—(Cl)]	C	−3.8	18.9	19.9175	2.47152	−25.0357	8.72649
		J	−15.9	79.08	83.3350	10.3408	−104.749	36.5116
26	[C_B—(Br)]	C	10.7	21.6	28.5533	2.26669	−23.2378	8.21083
		J	44.77	90.37	119.467	9.48383	−97.2270	34.3541
27	[C_B—(I)]	C	24.0	23.7	27.4198	2.50392	−28.4218	11.1429
		J	100.42	99.16	114.725	10.4764	−118.917	46.6219
28	[C—(C_B)(F)$_3$]	C	−162.7	42.8	−17.1592	6.57808	−68.7282	25.6714
		J	−680.74	179.08	−71.7939	27.5227	−287.559	107.409

1	[C—(H)$_3$(S)]	C	−10.08	30.41	−0.12863	2.35477	−10.1393	1.37028
		J	−42.17	127.24	−0.53818	9.85236	−42.4232	5.73325
2	[C—(C)(H)$_2$(S)]	C	−5.65	9.88	−10.3863	2.50400	−13.1644	3.31216
		J	−23.64	41.34	−43.4564	10.4767	−55.0798	13.8581
3	[C—(C)$_2$(H)(S)]	C	−2.64	−11.32	−30.7665	3.51939	−32.4716	10.9264
		J	−11.05	−47.36	−128.727	14.7251	−135.861	45.7161
4	[C—(C)$_3$(S)]	C	−0.55	−34.41	−36.6981	3.67289	−33.1473	8.20567
		J	−2.30	−143.97	−153.545	15.3674	−138.688	34.3325
5	[C$_B$—(S)]	C	−1.8	10.20	−44.4842	4.06530	−48.3650	19.0805
		J	−7.53	42.68	−186.122	17.0092	−202.359	79.8328
6	[C$_d$—(H)(S)]	C	8.56	8.0	10.6499	1.15719	−4.15581	−0.03040
		J	35.82	33.47	44.5592	4.84168	−17.3879	−0.12720
7	[C$_d$—(C)(S)]	C	10.93	−12.41	29.0382	0.20512	−0.85296	0.88804
		J	45.73	−51.92	121.496	0.85822	−3.56878	3.71556
8	[S—(C)(H)]	C	4.62	32.73	47.1743	0.41932	−1.27322	0.07441
		J	19.33	136.94	197.377	1.75443	−5.32715	0.31133
9	[S—(C$_B$)(H)]	C	11.96	12.66	61.4088	−0.81258	18.2174	−8.38456
		J	50.04	52.97	256.934	−3.39983	76.2216	−35.0810
10	[S—(C)$_2$]	C	11.51	13.15	57.0860	−0.42474	7.04715	−2.77241
		J	48.16	55.02	238.848	−1.77711	29.4853	−11.5998
11	[S—(C$_d$)$_2$]	C	−4.54	16.48	46.4150	−0.12876	7.57212	−1.16964
		J	−19.00	68.95	194.200	−0.53873	31.6818	−4.89377
12	[S—(S)(C)]	C	7.05	12.37	39.4952	0.64325	−8.01129	2.75383
		J	29.50	51.76	165.248	2.69136	−33.5192	11.5219
13	[S—(S)$_2$]	C	3.01	13.4	31.4964	0.77580	−9.75338	4.25273
		J	12.59	56.07	131.781	3.2460	−40.8081	17.7933
14	[C—(SO)(H)$_3$]	C	−10.08	30.41	−0.12858	2.35477	−10.1393	1.37028
		J	−42.17	127.24	−0.53797	9.85236	−42.4228	5.73333
15	[SO—(C)$_2$]	C	−14.41	18.10	21.9473	3.37991	−43.6119	18.8105
		J	−60.29	75.73	91.8275	14.1415	−182.472	78.7010
16	[C—(SO$_2$)(H)$_3$]	C	−10.08	30.41	−0.12858	2.35477	−10.1393	1.37028
		J	−42.17	127.24	−0.53797	9.85236	−42.4228	5.73333
17	[CO—(S)(C)]	C	−31.56	15.43	33.0893	0.71637	2.33423	−3.19742
		J	−132.05	64.56	138.446	2.99729	9.76642	−13.3780
18	[S—(H)(CO)]	C	−1.41	31.20	67.8808	0.33163	−0.59360	−1.25131
		J	−5.89	130.54	284.013	1.38754	−2.48362	−5.23548
19	[CS—(N)$_2$]	C	−31.56	15.43	33.0893	0.71637	2.33423	−3.19742
		J	−132.05	64.56	138.446	2.99729	9.76642	−13.3780
20	[N—(CS)(H)$_2$]	C	12.78	29.19	8.28988	2.27934	−19.6902	7.05934
		J	53.47	122.13	34.6849	9.53676	−82.3883	29.5363

No.	Group		ΔH^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$a \cdot 10$/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	$b \cdot 10^3$/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	$c \cdot 10^6$/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	$d \cdot 10^9$/ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
21		C	17.70	29.47	−66.1041	2.13517	−33.2547	12.6918
		J	74.06	123.30	−276.580	8.93355	−139.138	53.1025
22		C	19.37	27.18	−80.8421	1.73668	−21.1635	6.17446
		J	81.04	113.72	−338.243	7.26627	−88.5481	25.8339
23		C	1.73	23.56	−95.5376	2.14372	−22.9360	5.45174
		J	7.24	98.57	−399.729	8.96932	−95.9642	22.8101
24		C	0	16.10	−152.527	3.58279	−20.1302	0.82361
		J	0	67.36	−638.173	14.9904	−84.2248	3.44598
25		C	1.73	23.56	−95.5376	2.14372	−22.9360	5.45174
		J	7.24	98.57	−399.729	8.96932	−95.9642	22.8101
	Radicals							
1	[·C—(C)(H)$_2$]	C	35.82	30.7	4.99280	2.33523	−18.7613	6.38442
		J	149.87	128.45	20.8898	9.77060	−78.497	26.7124
2	[·C—(C)$_2$(H)]	C	37.45	10.74	10.7662	1.76526	−14.7999	4.92079
		J	156.69	44.94	45.0458	7.38585	−61.92278	20.5885
3	[·C—(C)$_3$]	C	38.00	−10.77	2.66049	1.72111	−16.4955	5.38030
		J	158.99	−45.06	11.1315	7.20112	−69.0172	22.5111
4	[C—(C·)(H)$_3$]	C	−10.08	30.41	−0.12858	−2.35477	−10.1393	1.37028
		J	−42.17	127.23	−0.53798	−9.85236	−42.4228	5.73325
5	[C—(C·)(C)(H)$_2$]	C	−4.95	9.42	−3.24681	2.32746	−13.9382	3.32919
		J	−20.71	39.41	−13.5846	9.73813	−58.3174	13.9293
6	[C—(C·)(C)$_2$(H)]	C	−1.9	−12.07	−20.2397	2.82589	−23.3851	7.21075
		J	−7.95	−50.50	−84.6829	11.8235	−97.8436	30.1697
7	[C—(C·)(C)$_3$]	C	1.50	−35.10	−50.1623	4.34818	−45.2765	15.5862
		J	6.28	−146.86	−209.879	18.1928	−189.436	65.2127
8	[C—(O·)(C)(H)$_2$]	C	6.1	36.4	34.0935	1.33337	8.84524	−9.18754
		J	25.52	152.30	142.647	5.57882	37.0085	−38.4406
9	[C—(O·)(C)$_2$(H)]	C	7.8	14.7	15.9068	2.34514	−9.65842	−0.88165
		J	32.63	61.50	66.5541	9.81207	−40.4108	−3.68882

10	[C—(O·)(C)$_3$]	C	8.6	−7.5	2.92515	2.95943	−22.5140	4.93680
		J	35.98	−31.38	12.2388	12.3823	−94.1986	20.6556
11	[C—(S·)(C)(H)$_2$]	C	32.4	39.0	22.3999	2.62896	−13.7331	2.60388
		J	135.56	163.18	93.7212	10.9996	−57.4593	10.8946
12	[C—(S·)(C)$_2$(H)]	C	35.5	17.8	9.66582	3.25478	−27.7056	8.80454
		J	148.53	74.47	40.4418	13.6180	−115.920	36.8382
13	[C—(S·)(C)$_3$]	C	37.5	−5.3	−25.8437	5.17183	−60.1663	23.3396
		J	156.9	−22.17	−108.130	21.6389	251.736	97.6529
14	[·C—(H)$_2$(C$_d$)]	C	23.2	27.65	−25.7771	3.52046	−32.1059	11.6677
		J	97.07	115.69	−107.851	14.7296	−134.331	48.8177
15	[·C—(H)(C)(C$_d$)]	C	25.5	7.02	−26.4802	3.25108	−31.1740	11.1074
		J	106.69	29.37	−110.793	13.6025	−130.432	46.4734
16	[·C—(C)$_2$(C$_d$)]	C	24.8	−15.0	4.26852	1.42912	−8.54900	0.87052
		J	103.76	−62.76	17.8595	5.97944	−35.7690	3.64226
17	[C$_d$—(C·)(H)]	C	8.59	7.97	10.6504	1.15718	−4.15446	−0.03038
		J	35.94	33.35	44.5612	4.84164	−17.3823	−0.12711
18	[C$_d$—(C·)(C)]	C	10.34	−12.3	16.1242	1.10092	−9.81452	3.38431
		J	43.26	−51.46	67.4636	4.60625	−41.0639	14.1599
19	[·C—(C$_B$)(H)$_2$]	C	23.0	26.85	0.21172	2.78887	−23.8078	8.31475
		J	96.23	112.34	0.88584	11.6692	−99.6210	34.7887
20	[·C—(C$_B$)(C)(H)]	C	24.7	6.36	−25.7428	3.67996	−39.3457	14.9808
		J	103.34	26.61	−107.708	15.3970	−164.622	62.6797
21	[·C—(C$_B$)(C)$_2$]	C	25.5	−15.46	8.61853	1.65135	−13.2960	3.02167
		J	106.69	−64.68	36.0599	6.90925	−55.6305	12.6399
22	[C$_B$—(C·)]	C	5.51	−7.69	14.0054	0.31667	4.57659	−3.70294
		J	23.05	−32.17	58.5986	1.32495	19.1484	−15.4931
23	[C—(·CO)(H)$_3$]	C	−5.4	66.6	69.1062	1.90829	2.79309	−5.51547
		J	−22.59	278.65	289.140	7.98428	11.6863	−23.0767
24	[C—(·CO)(C)(H)$_2$]	C	−0.3	45.8	68.6134	2.29656	−11.6016	2.50488
		J	−1.25	191.63	287.078	9.60881	−48.5428	10.4804
25	[C—(·CO)(C)$_2$(H)]	C	2.6	23.7	70.0112	1.45900	2.68747	−5.78530
		J	10.88	99.16	292.927	6.10446	11.2445	−24.2057
26	[·N—(H)(C)]	C	55.3	30.23	46.8484	0.22250	0.63835	−0.57315
		J	231.37	126.48	196.012	0.93090	2.67086	−2.39806
27	[·N—(C)$_2$]	C	58.4	10.24	20.6802	0.73017	−6.37086	1.96025
		J	244.34	42.84	86.5259	3.05503	−26.6556	8.20117
28	[C—(·N)(C)(H)$_2$]	C	−6.6	9.8	−18.9138	3.01262	−23.2942	7.40836
		J	−27.61	41.00	−79.1353	12.6048	−97.4629	30.9967
29	[C—(·N)(C)$_2$(H)]	C	−5.2	−11.7	−37.3690	3.82532	−38.2549	13.9859
		J	−21.75	−48.95	−156.352	16.0051	−160.058	58.5170
30	[C—(·N)(C)$_3$]	C	−3.2	34.1	−56.1025	4.75138	−53.4861	20.1061
		J	−13.39	142.67	−234.733	19.8798	−223.786	84.1239

No.	Group	Δ	H^0_{f298}/ kcal mol^{-1} or kJ mol^{-1}	S^0_{298}/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	a·10/ cal mol^{-1}K^{-1} or J mol^{-1}K^{-1}	b·10^2/ cal mol^{-1}K^{-2} or J mol^{-1}K^{-2}	c·10^6/ cal mol^{-1}K^{-3} or J mol^{-1}K^{-3}	d·10^9/ cal mol^{-1}K^{-4} or J mol^{-1}K^{-4}
31	[·C—(H)$_2$(CN)]	C	58.2	58.5	13.8803	3.97990	−32.9166	11.5435
		J	243.51	244.76	58.0752	16.6519	−137.723	48.2980
32	[·C—(H)(C)(CN)]	C	56.8	40.0	−11.5678	4.48052	−38.9246	12.6912
		J	237.65	167.36	−48.3997	18.7465	−162.861	53.0999
33	[·C—(C)$_2$(CN)]	C	56.1	19.6	28.3449	2.52852	−19.0188	5.41685
		J	234.72	82.01	118.595	10.5793	−79.5747	22.6641
34	[·N—(H)(C$_B$)]	C	38.0	27.3	12.1571	1.47162	−12.5532	4.33363
		J	158.99	114.22	50.8653	6.15726	−52.5226	18.1319
35	[·N—(C)(C$_B$)]	C	42.7	6.5	31.2852	0.10362	6.34074	−4.70402
		J	178.66	27.20	130.897	0.43355	26.5297	−19.6816
36	[C$_B$—(N·)]	C	−0.5	−9.69	35.7047	3.69427	−44.8486	18.0540
		J	−2.09	−40.54	149.388	15.4568	−187.647	75.5379
37	[C—(CO$_2$·)(H)$_3$]	C	−47.5	71.4	29.18647	4.29621	−14.6333	−1.63682
		J	−198.74	298.74	122.116	17.9753	−61.2257	−6.84845
38	[C—(CO$_2$·)(H)$_2$(C)]	C	−41.9	49.8	164.658	−2.63386	99.0545	−61.8602
		J	−175.31	208.36	688.929	−11.0201	414.444	−258.823
39	[C—(CO$_2$·)(H)(C)$_2$]	C	−39.0	−12.1	−24.5070	3.05694	−27.3758	9.37218
		J	−163.18	-50.63	−102.537	12.7902	−114.540	39.2132
40	[N$_A$—(N$_A$·)(C)]	C	74.2	36.1	62.9777	0.65357	−5.34247	1.51590
		J	310.4	151.04	263.499	2.73454	−22.3529	6.34253

Table II

Calculation of the ΔH_f^0 and S^0 functions and the parameters of eq.(1) from group contributions for 2-methylpentane

Groups	ΔH_f^0/ kJ mol^{-1}	S^0/ J mol^{-1}K^{-1}	$a\cdot 10$/ J mol^{-1}K^{-1}	$b\cdot 10^2$/ J mol^{-1}K^{-2}	$c\cdot 10^6$/ J mol^{-1}K^{-3}	$d\cdot 10^9$/ J mol^{-1}K^{-4}
[C—(C)(H)$_3$]	−42.1747	127.235	−0.537979	9.85248	−42.4216	5.73334
[C—(C)(H)$_3$]	−42.1747	127.235	−0.537979	9.85248	−42.4216	5.73334
[C—(C)(H)$_3$]	−42.1747	127.235	−0.537979	9.85248	−42.4216	5.73334
[C—(C)$_2$(H)$_2$]	−20.6271	39.4133	−13.5905	9.73826	−58.3300	13.9296
[C—(C)$_3$(H)]	−7.94960	−50.5009	−84.6831	11.8235	−97.8437	30.1697
Corrections	3.35					
1 gauche						
(−R ln 27)		−27.40				
Σ	−172.38	382.63	−113.478	60.8575	−341.768	75.2289
Experimental	−174.31	380.53	−127.429	63.0522	−378.610	92.0796

Table III

Application of the suggested method in the calculation of thermochemical quantities

Compound	Mode of calc.[a]	$a \cdot 10$/ $J\ mol^{-1}K^{-1}$	$b \cdot 10^2$/ $J\ mol^{-1}K^{-2}$	$c \cdot 10^6$/ $J\ mol^{-1}K^{-3}$	$d \cdot 10^9$/ $J\ mol^{-1}K^{-4}$	$\frac{C^0_{p\,1000}}{J\ mol^{-1}K^{-1}}$	$\frac{S^0_{1000}}{J\ mol^{-1}K^{-1}}$	$\frac{H^0_{1000}-H^0_{298}}{kJ\ mol^{-1}}$
Ethane	A	—	—	—	—	122.7	332.2	64.56
	B	81.8553	16.1441	−40.0309	−6.96267	123.6	332.8	65.02
	C	−1.07596	19.7050	−84.8432	11.4667	123.6	333.7	65.00
Propane	A	—	—	—	—	175.0	417.4	92.76
	B	−53.3136	31.0202	−164.579	34.6591	174.9	417.4	92.76
	C	−14.6665	29.4432	−143.173	25.3963	175.2	417.8	92.96
2-Methylpentane	A	—	—	—	—	331.4	664.9	178.24
	B	−127.429	63.0522	−378.610	92.0796	331.2	665.3	178.27
	C	−113.478	60.8575	−341.768	75.2289	331.2	667.4	177.00
Propene	A	—	—	—	—	144.2	390.2	77.24
	B	50.8950	22.5607	−99.8733	13.2829	144.1	390.2	77.24
	C	49.6284	22.8833	−105.335	15.9298	144.3	390.8	77.47
2-Methylpropene	A	—	—	—	—	196.0	463.1	105.9
	B	62.8179	32.5746	−171.960	35.9177	196.0	463.2	105.9
	C	94.3618	31.2903	−153.992	27.8283	196.2	462.8	106.1
Acetylene	A	—	—	—	—	66.61	268.2	40.58
	B	158.169	12.8122	−127.799	50.5659	66.71	268.1	40.54
	C	156.742	12.9346	−129.802	51.4174	66.64	268.2	40.50
Ethanol	A	—	—	—	—	141.5	405.8	76.90
	B	56.8192	23.5309	−125.797	26.4868	141.7	405.9	76.94
	C	66.0400	22.4116	−107.483	17.7382	141.0	402.8	76.20
Ethyl ether	A	—	—	—	—	244.8	554.0	132.04
	B	223.362	33.4103	−105.856	−5.95328	244.6	554.0	132.05
	C	−134.425	49.4279	−325.799	91.0474	246.1	560.6	132.60
1,2-Dichloroethane	A	—	—	—	—	138.1	438.9	80.00
	B	262.666	21.6347	−145.250	40.7194	138.1	438.9	79.96
	C	63.9822	29.1303	−239.588	81.6534	139.8	440.1	79.73
Ethanethiol	A	—	—	—	—	148.0	427.4	81.50
	B	141.213	23.1175	−125.255	27.9512	148.0	427.6	81.51
	C	153.383	22.0836	−102.829	19.9027	153.2	429.6	82.93

a A: critical data [4]
B: equation (1) from critical C^0_p of the compounds [1]
C: equation (1) from group additivities, present work

The calculated parameters (together with ΔH_f^0 and S^0 data for convenience) are collected in Table I. An example of the application of the collected data to calculate the thermochemical data of 2-methylpentane is shown in Table II, while some arbitrarily chosen examples to illustrate the reliability of the procedure applied are shown in Table III. In most cases the agreement is excellent.

It should be kept in mind that in some cases corrections must be applied when the $C_{p,T}^0$ values are estimated from groups [3]. In such cases the corrections also compiled in Table I must be applied to the calculation of the parameters.

Since the contributions collected in Table I were calculated from C_p^0 group values for the temperature range 298—1000 K, it is suggested that the derived quantities should also be used preferentially in this range. Minor extrapolations to higher temperatures result in moderately increased errors in the calculated thermochemical data (see the examples shown in Table III ref. 1 for some compounds).

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ТЕМПЕРАТУРНАЯ ЗАВИСИМОСТЬ ТЕРМОХИМИЧЕСКИХ ВЕЛИЧИН. ПАРАМЕТРЫ ПОЛИНОМА $C_{p,T}^0 = a+bT+cT^2+dT^3$ НА ОСНОВАНИИ ГРУППОВЫХ ВКЛАДОВ

Л. Шереш

Рассчитаны групповые вклады к определению параметров полинома $C_{p,T}^0 = a+bT+ +cT^2+dT^3$. Данный метод позволяет расширить применимость функции C_p^0, полученного из указанного полинома, для быстрого и точного расчёта температурной зависимости различных термохимических величин.