THREE DATASETS FROM THE PAPER *„MATRIX QUASI-NORMS AND NORMS AS MOLECULAR DESCRIPTORS"* BY PIOTR WILCZEK

QPRS studies on the standard enthalpy of formation (in gas phase, at 25℃, $\Delta_f H$) of alkanes

$$\Delta_f H = 36.36(\pm 2.0615) + 25.053(\pm 0.3252)(\|MM^2(G)\|_{0.625})^{\frac{1}{2}} \quad (Eq. 4)$$

$$n = 39\ R^2 0.9938\ s = 2.7398\ F = 5934.6\ Q^2 = 0.9929\ SDEP = 2.8476$$

Table 1. The values of topological indices from Eq. 4.

No.	Compound	$\|MM^2(G)\|_{0.625}$
1	ethane	3.0314
2	propane	7.7422
3	butane	13.5786
4	2-methylpropane	15.4272
5	pentane	20.4512
6	2-methylbutane	22.3132
7	2,2-dimethylpropane	26.3532
8	hexane	28.3275
9	2-methylpentane	30.3645
10	3-methylpentane	30.0615
11	2,3-dimethylbutane	32.2207
12	2,2-dimethylbutane	34.2233
13	heptane	37.1284
14	2-methylhexane	39.3783
15	3-methylhexane	38.9775
16	3-ethylpentane	38.5717
17	2,4-dimethylpentane	41.6419
18	2,2-dimethylpentane	43.5077
19	2,3-dimethylpentane	40.9905
20	3,3-dimethylpentane	42.8113
21	2,2,3-trimethylbutane	45.3663
22	octane	46.7928
23	2-methylheptane	49.2429
24	3-methylheptane	48.8070
25	4-methylheptane	48.7345
26	2,5-dimethylhexane	51.7397
27	3-ethylhexane	48.2932
28	2,4-dimethylhexane	51.2572
29	2,2-dimethylhexane	53.7226
30	2,3-dimethylhexane	50.9208
31	3,4-dimethylhexane	50.5289
32	3,3-dimethylhexane	52.8500
33	3-ethyl-2-methylpentane	50.4378
34	2,2,4-trimethylpentane	56.2364
35	2,3,4-trimethylpentane	53.1327
36	3-ethyl-3-methylpentane	52.0621
37	2,2,3-trimethylpentane	55.2374
38	2,3,3-trimethylpentane	54.8353
39	2,2,3,3-tetramethylbutane	59.8928

$$\Delta_f H = 191.5359(\pm 0.3809) - 210.436(\pm 2.3788)\frac{\|A(G)\|_{1.7}^{Sch}}{N} + 18.4077(\pm 2.3788)\left(\frac{\|A(G)\|_{1.7}^{Sch}}{N}\right)^2 \quad (Eq.5)$$

$$n = 39\ R^2 = 0.9955\ s = 2.3788\ F = 3942.93\ Q^2 = 0.9948\ SDEP = 2.4545$$

Table 2. The values of topological indices from Eq. 5.

No.	Compound	$\frac{\|A(G)\|_{1.7}^{Sch}}{N}$
1	ethane	0.7517
2	propane	0.7087
3	butane	0.6752
4	2-methylpropane	0.6510
5	pentane	0.6329
6	2-methylbutane	0.6256
7	2,2-dimethylpropane	0.6014
8	hexane	0.6013
9	2-methylpentane	0.5909
10	3-methylpentane	0.5982
11	2,3-dimethylbutane	0.5868
12	2,2-dimethylbutane	0.5822
13	heptane	0.5714
14	2-methylhexane	0.5659
15	3-methylhexane	0.5679
16	3-ethylpentane	0.5696
17	2,4-dimethylpentane	0.5569
18	2,2-dimethylpentane	0.5543
19	2,3-dimethylpentane	0.5639
20	3,3-dimethylpentane	0.5619
21	2,2,3-trimethylbutane	0.5517
22	octane	0.5473
23	2-methylheptane	0.5410
24	3-methylheptane	0.5449
25	4-methylheptane	0.5419
26	2,5-dimethylhexane	0.5369
27	3-ethylhexane	0.5455
28	2,4-dimethylhexane	0.5379
29	2,2-dimethylhexane	0.5343
30	2,3-dimethylhexane	0.5389
31	3,4-dimethylhexane	0.5431
32	3,3-dimethylhexane	0.5366
33	3-ethyl-2-methylpentane	0.5398
34	2,2,4-trimethylpentane	0.5265
35	2,3,4-trimethylpentane	0.5355
36	3-ethyl-3-methylpentane	0.5419
37	2,2,3-trimethylpentane	0.5329
38	2,3,3-trimethylpentane	0.5342
39	2,2,3,3-tetramethylbutane	0.5230

$$\Delta_f H = 279.9627(\pm 12.1230) - 5.6218(\pm 0.7705)\frac{\|RD(G)\|_{0.7}}{N} + 390.2379(\pm 24.8743)\|MM^2(G)\|_{0.675} - 32.1028(\|MM^2(G)\|_{0.675})^2 \quad (Eq.6)$$

$$n = 39\ R^2 = 0.9977\ s = 1.7179\ F = 5052.66\ Q^2 = 0.9971\ SDEP = 1.8255$$

Table 3. The values of topological indices from Eq. 6.

No.	Compound	$\frac{\|RD(G)\|_{0.7}}{N}$	$\|MM^2(G)\|_{0.675}$
1	ethane	1.3459	2.7924
2	propane	3.5436	6.4122
3	butane	6.1293	10.6498
4	2-methylpropane	6.4150	11.7885
5	pentane	8.9481	15.4552
6	2-methylbutane	9.3741	16.5603
7	2,2-dimethylpropane	9.9302	18.9207
8	hexane	11.9233	20.8071
9	2-methylpentane	12.4261	21.9829
10	3-methylpentane	12.5731	21.7982
11	2,3-dimethylbutane	12.9874	23.0426
12	2,2-dimethylbutane	13.2558	24.1721
13	heptane	15.0103	26.6507
14	2-methylhexane	15.5580	27.9234
15	3-methylhexane	15.7908	27.6818
16	3-ethylpentane	16.0246	27.4366
17	2,4-dimethylpentane	16.1384	29.1933
18	2,2-dimethylpentane	16.5387	30.2160
19	2,3-dimethylpentane	16.4241	28.8088
20	3,3-dimethylpentane	16.8265	29.8062
21	2,2,3-trimethylbutane	17.2319	31.2403
22	octane	18.1812	32.9452
23	2-methylheptane	18.7557	34.3072
24	3-methylheptane	19.0425	34.0489
25	4-methylheptane	19.1310	34.0042
26	2,5-dimethylhexane	19.3513	35.6871
27	3-ethylhexane	19.4194	33.7420
28	2,4-dimethylhexane	19.6667	35.4023
29	2,2-dimethylhexane	19.8254	36.7545
30	2,3-dimethylhexane	19.8046	35.2082
31	3,4-dimethylhexane	20.0324	34.9780
32	3,3-dimethylhexane	20.2820	36.2453
33	3-ethyl-2-methylpentane	20.1222	34.9218
34	2,2,4-trimethylpentane	20.4835	38.1267
35	2,3,4-trimethylpentane	20.5114	36.4194
36	3-ethyl-3-methylpentane	20.6510	35.7865
37	2,2,3-trimethylpentane	20.9029	37.5553
38	2,3,3-trimethylpentane	21.0433	37.3238
39	2,2,3,3-tetramethylbutane	21.8344	40.0767