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

QSPR studies on the boiling point (BP) of alkanes

$$BP = -182.8288(\pm 2.4295) + 62.9514(\pm 0.5751)\|A(G)\|_{1.55}^{Sch} \quad (Eq.\,1a)$$

$$n = 39\ R^2 = 0.9969\ s = 2.7661\ F = 11982.6\ Q^2 = 0.9964\ SDEP = 2.8938$$

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

Compound	$\|A(G)\|_{1.55}$
ethane	1.5639
propane	2.2117
butane	2.8844
2-methylpropane	2.7088
pentane	3.4069
2-methylbutane	3.3460
2,2-dimethylpropane	3.1278
hexane	3.9378
2-methylpentane	3.8214
3-methylpentane	3.9081
2,3-dimethylbutane	3.7806
2,2-dimethylbutane	3.7348
heptane	4.3956
2-methylhexane	4.3294
3-methylhexane	4.3548
3-ethylpentane	4.3763
2,4-dimethylpentane	4.2091
2,2-dimethylpentane	4.1802
2,3-dimethylpentane	4.3076
3,3-dimethylpentane	4.2850
2,2,3-trimethylbutane	4.1492
octane	4.8561
2-methylheptane	4.7619
3-methylheptane	4.8257
4-methylheptane	4.7739
2,5-dimethylhexane	4.7034
3-ethylhexane	4.8343
2,4-dimethylhexane	4.7193
2,2-dimethylhexane	4.6686
2,3-dimethylhexane	4.7337
3,4-dimethylhexane	4.8024
3,3-dimethylhexane	4.7034
3-ethyl-2-methylpentane	4.7470
2,2,4-trimethylpentane	4.5488
2,3,4-trimethylpentane	4.6870
3-ethyl-3-methylpentane	4.7878

2,2,3-trimethylpentane	4.6512
2,3,3-trimethylpentane	4.6702
2,2,3,3-tetramethylbutane	4.5024

$$BP = -365.8283(\pm 3.3769) - 214.7044(\pm 7.6967)\|A(G)\|_{3.025}^{Sch} + 435.701(\pm 9.6692)\|RD(G)\|_{3.025} \quad (Eq.\,2a)$$

$$n = 39\ R^2 = 0.9982\ s = 2.1312\ F = 10106.49\ Q^2 = 0.9978\ SDEP = 2.2526$$

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

Compound	$\|A(G)\|_{3.025}$	$\|RD(G)\|_{3.025}$
ethane	1.2575	1.2575
propane	1.7784	1.6128
butane	2.0707	1.8626
2-methylpropane	2.1781	1.8788
pentane	2.3069	2.0608
2-methylbutane	2.3758	2.0771
2,2-dimethylpropane	2.5150	2.1029
hexane	2.4980	2.2274
2-methylpentane	2.5636	2.2424
3-methylpentane	2.5479	2.2451
2,3-dimethylbutane	2.6132	2.2588
2,2-dimethylbutane	2.6623	2.2698
heptane	2.6656	2.3726
2-methylhexane	2.7202	2.3861
3-methylhexane	2.7121	2.3893
3-ethylpentane	2.7045	2.3925
2,4-dimethylpentane	2.7777	2.3999
2,2-dimethylpentane	2.8159	2.4120
2,3-dimethylpentane	2.7585	2.4046
3,3-dimethylpentane	2.7962	2.4166
2,2,3-trimethylbutane	2.8537	2.4285
octane	2.8129	2.5019
2-methylheptane	2.8637	2.5143
3-methylheptane	2.8536	2.5175
4-methylheptane	2.8588	2.5183
2,5-dimethylhexane	2.9104	2.5267
3-ethylhexane	2.8491	2.5215
2,4-dimethylhexane	2.9051	2.5303
2,2-dimethylhexane	2.9468	2.5383
2,3-dimethylhexane	2.8999	2.5324
3,4-dimethylhexane	2.8895	2.5352
3,3-dimethylhexane	2.9358	2.5439
3-ethyl-2-methylpentane	2.8949	2.5360
2,2,4-trimethylpentane	2.9969	2.5512
2,3,4-trimethylpentane	2.9412	2.5467
3-ethyl-3-methylpentane	2.9202	2.5488
2,2,3-trimethylpentane	2.9772	2.5574

2,3,3-trimethylpentane	2.9716	2.5595
2,2,3,3-tetramethylbutane	3.0574	2.5806

$$BP = -430.7251(\pm 16.9782) - 384.3954(\pm 44.2421)\|A(G)\|_{3.025}^{Sch} + 690.5543(\pm 66.2282)\|RD(G)\|_{3.025} - 68.9278(\pm 17.7743)log\left(\|MM^2(G)\|_{1.1}^{Sch}\right) \quad (Eq.\,3a)$$

$$n = 39\ R^2 = 0.9988\ s = 1.8076\ F = 9370.09\ Q^2 = 0.9984\ SDEP = 1.9374$$

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

Compound	$\|A(G)\|_{3.025}$	$\|RD(G)\|_{3.025}$	$\|MM^2(G)\|_{1.1}^{Sch}$
ethane	1.2575	1.2575	1.8779
propane	1.7784	1.6128	1.8779
butane	2.0707	1.8626	2.2936
2-methylpropane	2.1781	1.8788	1.8779
pentane	2.3069	2.0608	2.7148
2-methylbutane	2.3758	2.0771	2.4409
2,2-dimethylpropane	2.5150	2.1029	1.8779
hexane	2.4980	2.2274	3.1052
2-methylpentane	2.5636	2.2424	2.8560
3-methylpentane	2.5479	2.2451	2.9956
2,3-dimethylbutane	2.6132	2.2588	2.6314
2,2-dimethylbutane	2.6623	2.2698	2.5150
heptane	2.6656	2.3726	3.4980
2-methylhexane	2.7202	2.3861	3.2399
3-methylhexane	2.7121	2.3893	3.3977
3-ethylpentane	2.7045	2.3925	3.5564
2,4-dimethylpentane	2.7777	2.3999	2.9932
2,2-dimethylpentane	2.8159	2.4120	2.9270
2,3-dimethylpentane	2.7585	2.4046	3.1812
3,3-dimethylpentane	2.7962	2.4166	3.1402
2,2,3-trimethylbutane	2.8537	2.4285	2.7261
octane	2.8129	2.5019	3.8805
2-methylheptane	2.8637	2.5143	3.6321
3-methylheptane	2.8536	2.5175	3.7758
4-methylheptane	2.8588	2.5183	3.7928
2,5-dimethylhexane	2.9104	2.5267	3.3738
3-ethylhexane	2.8491	2.5215	3.9361
2,4-dimethylhexane	2.9051	2.5303	3.5317
2,2-dimethylhexane	2.9468	2.5383	3.3077
2,3-dimethylhexane	2.8999	2.5324	3.5789
3,4-dimethylhexane	2.8895	2.5352	3.7207
3,3-dimethylhexane	2.9358	2.5439	3.5411
3-ethyl-2-methylpentane	2.8949	2.5360	3.7386
2,2,4-trimethylpentane	2.9969	2.5512	3.0620
2,3,4-trimethylpentane	2.9412	2.5467	3.3641
3-ethyl-3-methylpentane	2.9202	2.5488	3.7582
2,2,3-trimethylpentane	2.9772	2.5574	3.2737
2,3,3-trimethylpentane	2.9716	2.5595	3.3467
2,2,3,3-tetramethylbutane	3.0574	2.5806	2.8305

$$BP = -169.7488(\pm 2.1037) + 56.9579(\pm 0.4795)\|A(G)\|_{1.475}^{Sch} \quad (Eq.1b)$$

$$n = 40\ R^2 = 0.9973\ s = 3.2491\ F = 14112.02\ Q^2 = 0.9964\ SDEP = 3.6514$$

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

No.	Compound	$\|A(G)\|_{1.475}^{Sch}$
1	methane	0.0000
2	ethane	1.5999
3	propane	2.2626
4	butane	2.9981
5	2-methylpropane	2.7711
6	pentane	3.5562
7	2-methylbutane	3.4809
8	2,2-dimethylpropane	3.1998
9	hexane	4.1444
10	2-methylpentane	3.9910
11	3-methylpentane	4.1089
12	2,3-dimethylbutane	3.9409
13	2,2-dimethylbutane	3.8843
14	heptane	4.6436
15	2-methylhexane	4.5598
16	3-methylhexane	4.5929
17	3-ethylpentane	4.6207
18	2,4-dimethylpentane	4.4001
19	2,2-dimethylpentane	4.3647
20	2,3-dimethylpentane	4.5338
21	3,3-dimethylpentane	4.5068
22	2,2,3-trimethylbutane	4.3266
23	octane	5.1584
24	2-methylheptane	5.0332
25	3-methylheptane	5.1214
26	4-methylheptane	5.0488
27	2,5-dimethylhexane	4.9592
28	3-ethylhexane	5.1322
29	2,4-dimethylhexane	4.9798
30	2,2-dimethylhexane	4.9155
31	2,3-dimethylhexane	4.9985
32	3,4-dimethylhexane	5.0933
33	3,3-dimethylhexane	4.9608
34	3-ethyl-2-methylpentane	5.0156
35	2,2,4-trimethylpentane	4.7557
36	2,3,4-trimethylpentane	4.9396
37	3-ethyl-3-methylpentane	5.0760
38	2,2,3-trimethylpentane	4.8947
39	2,3,3-trimethylpentane	4.9195
40	2,2,3,3-tetramethylbutane	4.6988

$$BP = -162.1545(\pm 2.4701) + 56.0672(\pm 0.4463)\|A(G)\|_{1.475}^{Sch} - 24.3899(\pm 5.6388)\frac{\|MM^2(G)\|_{4.425}}{N} \quad (Eq.\,2b)$$

$$n = 40\ R^2 = 0.9982\ s = 2.6834\ F = 10353.69\ Q^2 = 0.9969\ SDEP = 3.3831$$

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

No.	Compound	$\|A(G)\|_{1.475}^{Sch}$	$\frac{\|MM^2(G)\|_{4.425}}{N}$
1	methane	0.0000	0.0000
2	ethane	1.5999	0.5848
3	propane	2.2626	0.3464
4	butane	2.9981	0.2343
5	2-methylpropane	2.7711	0.2538
6	pentane	3.5562	0.1902
7	2-methylbutane	3.4809	0.1876
8	2,2-dimethylpropane	3.1998	0.2015
9	hexane	4.1444	0.1608
10	2-methylpentane	3.9910	0.1624
11	3-methylpentane	4.1089	0.1543
12	2,3-dimethylbutane	3.9409	0.1562
13	2,2-dimethylbutane	3.8843	0.1584
14	heptane	4.6436	0.1396
15	2-methylhexane	4.5598	0.1410
16	3-methylhexane	4.5929	0.1377
17	3-ethylpentane	4.6207	0.1369
18	2,4-dimethylpentane	4.4001	0.1427
19	2,2-dimethylpentane	4.3647	0.1419
20	2,3-dimethylpentane	4.5338	0.1348
21	3,3-dimethylpentane	4.5068	0.1332
22	2,2,3-trimethylbutane	4.3266	0.1358
23	octane	5.1584	0.1237
24	2-methylheptane	5.0332	0.1248
25	3-methylheptane	5.1214	0.1221
26	4-methylheptane	5.0488	0.1247
27	2,5-dimethylhexane	4.9592	0.1259
28	3-ethylhexane	5.1322	0.1240
29	2,4-dimethylhexane	4.9798	0.1236
30	2,2-dimethylhexane	4.9155	0.1256
31	2,3-dimethylhexane	4.9985	0.1224
32	3,4-dimethylhexane	5.0933	0.1186
33	3,3-dimethylhexane	4.9608	0.1223
34	3-ethyl-2-methylpentane	5.0156	0.1228
35	2,2,4-trimethylpentane	4.7557	0.1271
36	2,3,4-trimethylpentane	4.9396	0.1204
37	3-ethyl-3-methylpentane	5.0760	0.1185
38	2,2,3-trimethylpentane	4.8947	0.1204
39	2,3,3-trimethylpentane	4.9195	0.1182
40	2,2,3,3-tetramethylbutane	4.6988	0.1205

$$BP = -163.5355(\pm.3817) + 56.8971(\pm 0.5364)\|A(G)\|_{1.475}^{Sch} - 25.9714(\pm 5.3239)\frac{\|MM^2(G)\|_{4.425}}{N} - 0.012(\pm 0.0048)\|MM(G)\|_{0.325}^{Sch} \quad (Eq.3b)$$

$$n = 40\ R^2 = 0.9985\ s = 2.5152\ F = 7858.25\ Q^2 = 0.9981\ SDEP = 2.6842$$

Table 6. The experimental (Exptl) and calculated (Calcd) from Eq. 3b boiling points of 40 alkanes as well as the corresponding residual values (Res).

No.	Pt.*		BP(℃)		
			Exptl	Calcd	Res
1	A	methane	-164	-163.535	-0.465
2	B	ethane	-88.630	-87.796	-0.834
3	A	propane	-42.070	-43.902	1.832
4	C	butane	-0.500	0.335	-0.835
5	B	2-methylpropane	-11.730	-12.568	0.838
6	B	pentane	36.074	33.119	2.955
7	B	2-methylbutane	27.852	28.968	-1.116
8	A	2,2-dimethylpropane	9.503	13.178	-3.675
9	A	hexane	68.740	66.118	2.622
10	A	2-methylpentane	60.271	58.545	1.726
11	B	3-methylpentane	63.282	64.178	-0.896
12	A	2,3-dimethylbutane	57.988	55.897	2.091
13	B	2,2-dimethylbutane	49.741	52.646	-2.905
14	B	heptane	98.427	94.721	3.706
15	A	2-methylhexane	90.052	90.157	-0.105
16	C	3-methylhexane	91.850	91.901	-0.051
17	B	3-ethylpentane	93.475	93.350	0.125
18	C	2,4-dimethylpentane	80.500	82.297	-1.797
19	C	2,2-dimethylpentane	79.197	80.312	-1.115
20	A	2,3-dimethylpentane	89.784	88.743	1.041
21	A	3,3-dimethylpentane	86.064	87.216	-1.152
22	C	2,2,3-trimethylbutane	80.882	78.342	2.540
23	B	octane	125.655	122.181	3.474
24	C	2-methylheptane	117.647	117.182	0.465
25	C	3-methylheptane	118.925	119.987	-1.062
26	A	4-methylheptane	117.709	117.936	-0.227
27	B	2,5-dimethylhexane	109.103	113.162	-4.059
28	B	3-ethylhexane	118.534	120.511	-1.977
29	C	2,4-dimethylhexane	109.429	114.203	-4.774
30	A	2,2-dimethylhexane	106.840	110.739	-3.899
31	C	2,3-dimethylhexane	115.607	115.249	0.358
32	B	3,4-dimethylhexane	117.725	118.316	-0.591
33	A	3,3-dimethylhexane	111.969	113.118	-1.149
34	A	3-ethyl-2-methylpentane	115.650	116.081	-0.431
35	C	2,2,4-trimethylpentane	99.238	102.909	-3.671
36	C	2,3,4-trimethylpentane	113.467	112.083	1.384
37	A	3-ethyl-3-methylpentane	118.259	117.266	0.993
38	C	2,2,3-trimethylpentane	109.840	109.587	0.253
39	C	2,3,3-trimethylpentane	114.760	110.966	3.794
40	B	2,2,3,3-tetramethylbutane	106.470	99.883	6.587

* Pt. denotes the part (i.e., the subset A or B or C) in the external validation.

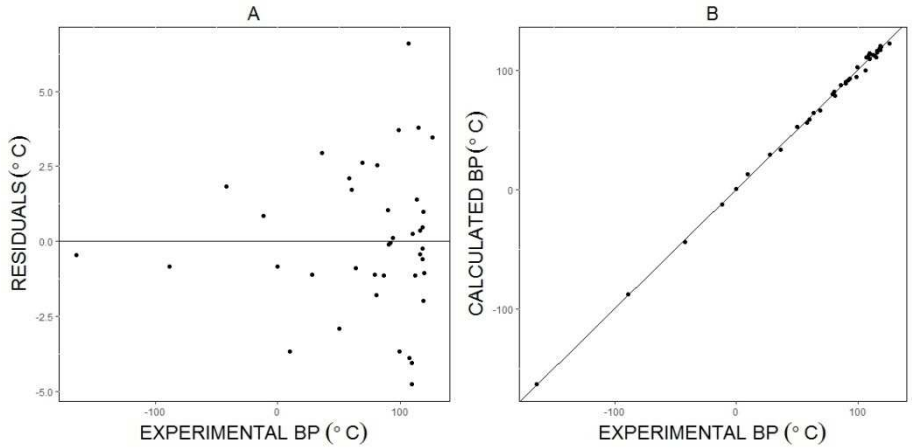

Figure 1. A – Plot of the experimental BP of 39 alkanes *vs.* the residuals of Eq. 3b, B – Plot of the experimental BP of 39 alkanes *vs.* the calculated (from Eq. 3b) values.

Table 7. The values of topological indices from Eq. 3b.

No.	Compound	$\|\|A(G)\|\|_{1.475}^{Sch}$	$\frac{\|\|MM^2(G)\|\|_{4.425}}{N}$	$\|\|MM(G)\|\|_{0.325}^{Sch}$
1	methane	0.0000	0.0000	0.0000
2	ethane	1.5999	0.5848	8.4381
3	propane	2.2626	0.3464	8.6041
4	butane	2.9981	0.2343	52.2701
5	2-methylpropane	2.7711	0.2538	8.8599
6	pentane	3.5562	0.1902	61.8330
7	2-methylbutane	3.4809	0.1876	56.6205
8	2,2-dimethylpropane	3.1998	0.2015	9.1175
9	hexane	4.1444	0.1608	164.9990
10	2-methylpentane	3.9910	0.1624	65.0019
11	3-methylpentane	4.1089	0.1543	172.0699
12	2,3-dimethylbutane	3.9409	0.1562	61.3764
13	2,2-dimethylbutane	3.8843	0.1584	59.0665
14	heptane	4.6436	0.1396	193.8299
15	2-methylhexane	4.5598	0.1410	173.7887
16	3-methylhexane	4.5929	0.1377	192.4564
17	3-ethylpentane	4.6207	0.1369	205.4397
18	2,4-dimethylpentane	4.4001	0.1427	67.9392
19	2,2-dimethylpentane	4.3647	0.1419	67.0343
20	2,3-dimethylpentane	4.5338	0.1348	181.8823
21	3,3-dimethylpentane	4.5068	0.1332	184.4181
22	2,2,3-trimethylbutane	4.3266	0.1358	64.0301
23	octane	5.1584	0.1237	381.2984
24	2-methylheptane	5.0332	0.1248	201.6528
25	3-methylheptane	5.1214	0.1221	392.0481
26	4-methylheptane	5.0488	0.1247	212.7811
27	2,5-dimethylhexane	4.9592	0.1259	182.9524
28	3-ethylhexane	5.1322	0.1240	395.2219
29	2,4-dimethylhexane	4.9798	0.1236	199.0994
30	2,2-dimethylhexane	4.9155	0.1256	178.7562
31	2,3-dimethylhexane	4.9985	0.1224	203.0763

32	3,4-dimethylhexane	5.0933	0.1186	405.4099
33	3,3-dimethylhexane	4.9608	0.1223	202.4949
34	3-ethyl-2-methylpentane	5.0156	0.1228	214.0370
35	2,2,4-trimethylpentane	4.7557	0.1271	69.8840
36	2,3,4-trimethylpentane	4.9396	0.1204	192.0425
37	3-ethyl-3-methylpentane	5.0760	0.1185	411.3507
38	2,2,3-trimethylpentane	4.8947	0.1204	187.3185
39	2,3,3-trimethylpentane	4.9195	0.1182	194.9500
40	2,2,3,3-tetramethylbutane	4.6988	0.1205	66.7903