

Regular article

Prediction of ^{13}C NMR chemical shifts in substituted naphthalenes

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Abstract. The prediction of the ^{13}C NMR signals for derivatives of naphthalene has been investigated using mathematical modeling techniques. Two empirical multiple regression models which utilize the field, resonance, and Charton's steric parameters together with molar refractivity were developed, one for α - and the other for β -substituted naphthalene derivatives. In the α case the model had a correlation coefficient of observed versus predicted line positions of $r = 0.973$ with a standard deviation of 2.2 ppm while in the β case $r = 0.979$ with the standard deviation being 2.3 ppm. The database consisted of 3152 signals from 394 naphthalene derivatives. We also report the use of the Taft steric parameter in place of the Charton steric parameter in the above-mentioned prediction equations.

Key words: ^{13}C NMR of naphthalenes – mathematical modeling

1 Introduction

We have investigated two different techniques that can be used to predict the NMR line positions using statistical methods. The first method is to use the statistical substituent chemical shift (SSCS) values. An SSCS value is a measure of the shift in an NMR line position induced by substituting a particular group on a structure which acts as a standard. We have reported SSCS values for a number of systems: the ^{11}B NMR spectra of trigonal boranes [1], the ^{13}C NMR spectra of arenes [2–3], and the ^{19}F NMR signals for fluoro derivatives of arenes [4], six-membered aromatic nitrogen heterocycles [5], arenetricarbonylchromium(0) complexes [6], and ethylenes [7].

The second technique is to establish an equation using known parameter values for the electronic, steric,

or polarization properties of the groups attached to the base structure in order to provide an estimate of the NMR line position. We have had success using the values for the field, resonance, and Charton's steric parameters (ν) together with molar refractivity (MR) in the prediction of the ^{11}B NMR of trigonal boranes [8], the ^{13}C NMR of arenes [9–10], the nitrogen NMR spectra for derivatives of ammonia [11–12], and the ^{19}F NMR signals for fluoroarenes [13–14] and fluoroarenetricarbonyl-chromium(0) complexes [15–16].

The studies reporting the ^{13}C NMR spectra [10] and the ^{19}F NMR spectra [14] of arenes were done utilizing symmetrical coefficients in the prediction equations, a technique which does not require any arbitrary orientation of the molecule before the prediction equation can be employed. In the above-mentioned older studies some arbitrary orientation of the molecule was necessary before the prediction equations could be employed which led to asymmetrical prediction equations.

In the present paper we report the application of the parameter method to the ^{13}C NMR spectra of substituted naphthalenes.

2 Experimental

Statistical computations were done on a Sun SPARC-10 using Statistical Analysis System (SAS) and on a Pentium Pro 200 computer running the Linux operating system.

3 Results and discussion

3.1 The database

We surveyed the literature from the period from 1970 until 1985. From this we extracted our database in which

1. The compound was a naphthalene derivative containing one or more groups. The groups are listed in Table 1.
2. All signals were converted so as to use tetramethylsilane as a reference. The database consists of 3152 signals from 394 naphthalene derivatives.

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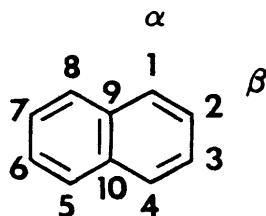
Table 1. Group numbers, codes, groups, field (F), resonance (R), steric parameters (v), and molar refractivity (MR) [17–19]^a

No.	Code	Group	F	R	v	MR
1	–	H	0.00	0.00	0.00	0.00
2	A	Br	0.44	–0.17	0.65	8.88
3	B	Cl	0.41	–0.15	0.55	6.03
4	C	NH ₂	0.02	–0.68	0.35	5.42
5	D	CH ₂ CH ₃	–0.05	–0.10	0.56	10.30
6	E	F	0.43	–0.34	0.27	0.92
8	F	OH	0.29	–0.64	0.32	2.85
11	G	OCH ₃	0.26	–0.51	0.36	7.87
12	I	CH ₃	–0.04	–0.13	0.52	5.65
13	J	NO ₂	0.67	0.16	0.59	7.36
14	K	SCH ₃	0.20	–0.18	0.64	13.82
15	L	COCH ₃	0.32	0.20	0.50	11.18
16	M	CH(CH ₃) ₂	–0.05	–0.10	0.76	14.96
17	N	C(CH ₃) ₃	–0.07	–0.13	1.24	19.62
18	P	N(CH ₃) ₂	0.10	–0.92	0.43	15.55
21	Q	CH ₂ OH	0.00	0.00	0.53	7.19
22	R	CH=CH ₂	0.07	–0.08	1.31	10.99
156	S	COOEt	0.33	0.15	0.69	17.47

^a We have used the same group numbers as in our previous papers [1–16] for consistency. The group codes are used for brevity in Table 4

3.2 Statistical analysis

Because of the geometry of the naphthalene molecule, there are three categories of ¹³C NMR signal, the α signals from carbons in positions 1, 4, 5, and 8 and the β signals from the carbons in positions 2, 3, 6, and 7. In addition there are also signals from the carbons in positions 9 and 10. This necessitates dividing the signals into three populations before models for prediction of the ¹³C NMR signals are computed. Thus we derive one model for predicting α signals and another model for predicting β signals. The signals from the carbons in positions 9 and 10 are nearly constant at around 130 ppm, and we were not successful in computing a model to accurately predict these signals.



For the α population each atom has four encodings in the file used to compute the model, one for each of the four α signals. The encoding is determined by orienting the atom so that the carbon with which the signal is associated is in position 1. The subscripts in the model refer to the numbered positions after this orientation has been made. For example, compound number 25, 1-acetyl-2-fluoronaphthalene has the following four encodings in the database used for computing the model for α signals.

15	6	1	1	1	1	1	121.6
1	1	6	15	1	1	1	131.7
1	1	1	1	15	6	1	127.0
1	1	1	1	1	1	6	123.5

The integers in the encoding refer to the substituent numbers, 6 being fluorine, 15 being acetyl, and 1 being hydrogen. The numbers for the substituents can be found in Table 1. The signals at the end of the line are from the carbons in position 1. The 394 compounds used in the study thus resulted in a database of 1576 alpha signals from which the model was computed.

There seems to be little interaction between adjacent groups. This may result partly from the fact that the compounds in this database are sparsely substituted. The small interactions between adjacent substituents means that the signals can probably be predicted well from SCS values, though very few SCS values can be determined directly from this database.

The variables used in the model are the field parameter, F , the resonance parameter, R , Charton's steric parameter, v , and MR. A scarcity of well determined values of v limits somewhat the compounds which can be predicted by this method. In the model, F_i , R_i , v_i , and MR_i denote the field, resonance, steric and molar refractivity respectively of the substituent in the i th position, $i = 1 \dots 8$. The model does not allow for interactions between different substituents, though it does seem to require self-interaction of parameters for the same substituent for substituents that are close to the signal being predicted. For α signals self-interaction variables are used for substituents in positions 1, 2, and 8. The coefficients of the variables were determined by stepwise multiple regression, and all variables statistically significant at the 5% level of significance were retained in the model resulting in 40 predictor variables including the self-interaction variables in positions 1, 2, and 8. The predicted variable δ is of course the ¹³C NMR shift of the carbon in position 1.

$$\begin{aligned}
 \delta = & 127.8 + 70.688 F_1 - 27.220 R_1 - 190.72 v_1 \\
 & + 14.559 MR_1 + 196.55 F_1 F_1 - 42.834 F_1 R_1 \\
 & - 231.76 F_1 v_1 - 5.4626 F_1 MR_1 + 7.2224 R_1 R_1 \\
 & + 4.2965 R_1 MR_1 + 306.69 v_1 v_1 - 21.318 v_1 MR_1 \\
 & - 41.976 F_2 + 130.39 R_2 + 6.3531 v_2 + 52.800 F_2 F_2 \\
 & - 27.970 F_2 R_2 + 25.485 F_2 v_2 + 31.497 R_2 R_2 \\
 & - 280.57 R_2 v_2 + 2.6142 R_2 MR_2 - 21.843 v_2 v_2 \\
 & + 3.6858 F_3 - 1.4474 R_3 - 0.041267 MR_3 \\
 & + 2.3903 F_4 + 12.594 R_4 - 2.3766 v_4 + 0.19569 MR_4 \\
 & + 1.8180 F_7 + 2.4424 R_7 - 0.69286 v_7 - 13.854 F_8 \\
 & + 33.238 R_8 - 6.9343 v_8 + 8.6060 F_8 F_8 + 18.478 F_8 v_8 \\
 & + 8.0666 R_8 R_8 - 83.349 R_8 v_8 + 0.50051 R_8 MR_8 \quad (1)
 \end{aligned}$$

Note that none of the variables in positions 5 and 6 were statistically significant which means that the signal for position 1 is scarcely influenced at all by the substituents in positions 5 and 6. The correlation of observed versus predicted signals, shown in Fig. 1, has a correlation

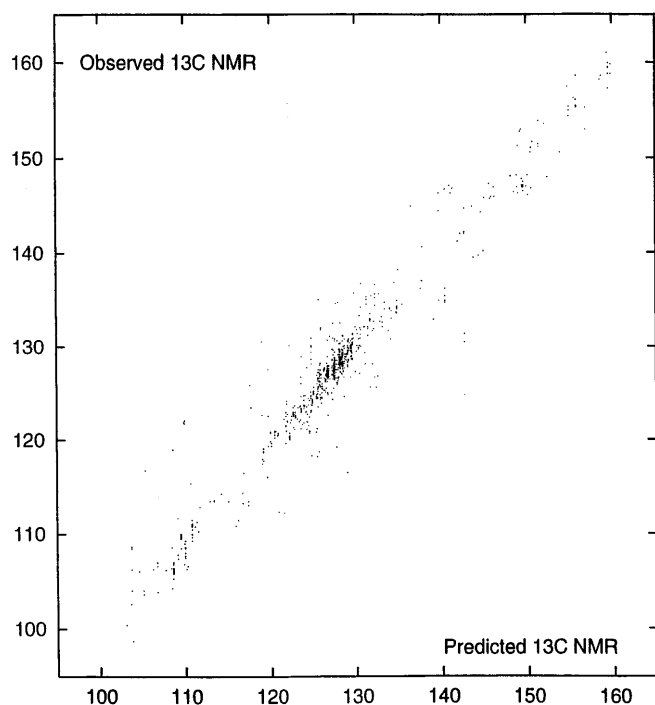


Fig. 1. Correlation between 1576 pairs of observed and predicted α signals. $r = 0.973$

coefficient of $r = 0.973$ with a standard deviation of 2.2 ppm. The average absolute error of prediction is therefore 1.5 ppm. Standard errors of estimate of the coefficients as well as p values are given in Table 2. The F value for the model was 682.5 which yields a p value under 0.0001. Most of the predictions with large residuals are from carbons with an attached amino group, though most carbons with an amino group attached are predicted quite accurately. We are unable to explain this anomaly.

To assess the internal validity of the model, we ran the leave-one-out cross-validation procedure. The sum of squares of errors (SSE) for the generated pseudovalues (PRESS) was 8438, only slightly higher than 7769, the (SSE) for the model. This indicates that the model ought to predict new data of similar type about as well as it predicts the data from which the model was generated.

In the database used for computing the model to predict β signals, the encodings are the same as for the α database except that the ^{13}C NMR signal listed at the end of a line is from the carbon in position 2. This results in the following four lines in this database for 1-acetyl-2-fluoronaphthalene, one line for each β signal.

15	6	1	1	1	1	1	1	156.8
1	1	6	15	1	1	1	1	114.5
1	1	1	1	15	6	1	1	124.4
1	1	1	1	1	1	6	15	127.0

As with α signals this complete database from which the prediction model was computed, has 1576 lines. Also F_i , R_i , v_i , and MR_i , $i = 1..8$ are defined as in the α model. For β signals we used self-interaction among the parameters for positions 1, 2, and 3. The model, determined by a stepwise regression procedure, has 39 variables significant at the 5% level.

Table 2. Variables, coefficient estimates, standard errors of estimates and p values of the estimates for the α -signal prediction model

Variable	Coefficient	Standard error	p value
Intercept	127.796964	0.10	0.0001
F_1	70.688176	7.86	0.0001
R_1	-27.219545	3.14	0.0001
v_1	-190.718670	15.97	0.0001
MR_1	14.559313	1.18	0.0001
F_1F_1	196.551886	8.69	0.0001
F_1R_1	-42.834403	9.24	0.0001
F_1v_1	-231.760136	21.63	0.0001
$F_1\text{MR}_1$	-5.462625	1.39	0.0001
R_1R_1	7.222446	3.57	0.0435
$R_1\text{MR}_1$	4.296523	0.41	0.0001
v_1v_1	306.693001	25.10	0.0001
$v_1\text{MR}_1$	-21.318317	1.68	0.0001
F_2	-41.975695	5.31	0.0001
R_2	130.389618	8.57	0.0001
v_2	6.353103	1.18	0.0001
F_2F_2	52.800189	5.71	0.0001
F_2R_2	-27.970103	6.04	0.0001
F_2v_2	25.485201	7.79	0.0011
R_2R_2	31.496608	3.67	0.0001
R_2v_2	-280.572438	21.65	0.0001
$R_2\text{MR}_2$	2.614244	0.19	0.0001
v_2v_2	-21.842650	2.15	0.0001
F_3	3.685843	0.50	0.0001
R_3	-1.447448	0.39	0.0003
MR_3	-0.041267	0.02	0.0423
F_4	2.390331	0.57	0.0001
R_4	12.594249	0.41	0.0001
v_4	-2.376637	0.86	0.0062
MR_4	0.195692	0.05	0.0002
F_7	1.818020	0.54	0.0008
R_7	2.442354	0.40	0.0001
v_7	-0.692858	0.34	0.0468
F_8	-13.854076	2.68	0.0001
R_8	33.237588	5.49	0.0001
v_8	-6.934299	0.76	0.0001
F_8F_8	8.605972	3.90	0.0277
F_8v_8	1.477871	4.98	0.0002
R_8R_8	8.066649	3.01	0.0075
R_8v_8	-83.348659	13.72	0.0001
$R_8\text{MR}_8$	0.500505	0.19	0.0099

$$\begin{aligned}
 \delta = & 126.54 - 17.415 F_1 + 161.04 R_1 + 46.617 F_1F_1 \\
 & + 12.289 F_1R_1 + 40.675 R_1R_1 - 387.55 R_1v_1 \\
 & + 3.0365 R_1\text{MR}_1 - 23.103 v_1v_1 + 26.377 F_2 \\
 & - 338.06 R_2 + 20.681 v_2 - 119.55 F_2F_2 \\
 & - 51.866 F_2R_2 + 93.790 F_2v_2 - 6.3687 F_2\text{MR}_2 \\
 & - 81.079 R_2R_2 + 971.80 R_2v_2 - 10.142 R_2\text{MR}_2 \\
 & + 56.138 v_2v_2 - 42.203 F_3 + 17.351 v_3 \\
 & - 0.46576 \text{MR}_3 - 55.468 F_3F_3 - 37.592 F_3R_3 \\
 & + 132.59 F_3v_3 - 2.9597 F_3\text{MR}_3 + 72.538 R_3v_3 \\
 & - 1.3890 R_3\text{MR}_3 - 1.7734 F_4 - 1.2537 R_4 \\
 & + 2.8366 F_5 + 1.0181 R_5 - 0.075999 \text{MR}_5 \\
 & + 2.1966 F_6 + 5.1689 R_6 + 3.3826 F_8 + 2.5651 R_8 \\
 & + 2.7794 v_8 - 0.13394 \text{MR}_8
 \end{aligned} \tag{2}$$

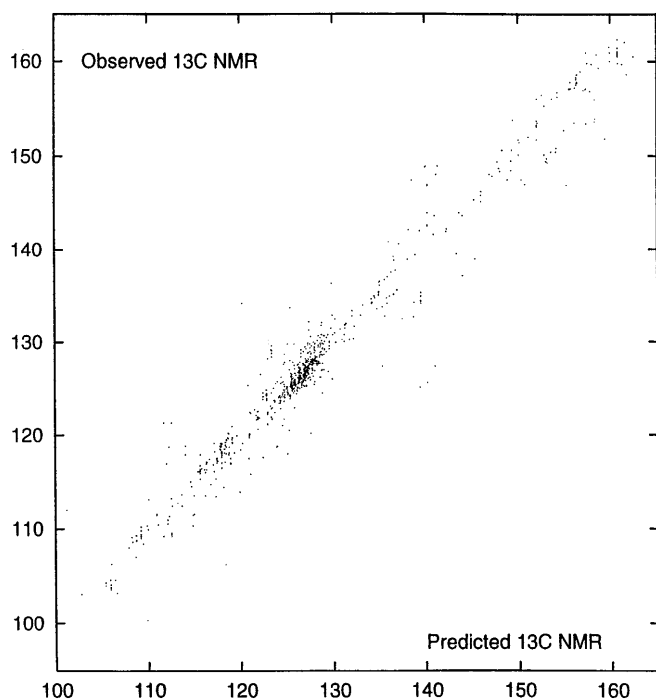


Fig. 2. Correlation between 1576 pairs of observed and predicted β signals. $r = 0.979$

The correlation of observed versus predicted signals, shown in Fig. 2, has a correlation coefficient of $r = 0.979$ with a standard deviation of $s = 2.3$ ppm. The average absolute error of prediction is 1.5 ppm. Standard errors of estimate for the coefficients as well as p values are given in Table 3. The F value for the model was 1000.0 which yields a p value under 0.0001. For β signals the variables in position 7 are not statistically significant, and thus the substituent in position 7 has a negligible effect on the signal from the carbon in position 2.

The take-one-out cross-validation procedure yields $SSE = 7810$ and $PRESS = 8479$. This represents only a small increase in SSE for the pseudovalues.

The 394 compounds used in this study are given in Table 4. This table lists the substituents in positions 1–8 as well as the observed and predicted NMR signals from these positions. Because Table 4 contains a large amount of data, for brevity we omitted signals 9 and 10, which we were unable to predict and encoded the compounds with a letter code rather than with the group numbers. The group numbers are also retained in this paper for consistency with our earlier papers in which we used these numbers.

3.3 Comparison of Taft and Charton steric factors in the above models

The advantage of the parameter method outlined above is that the number of variables is kept to a minimum; however there are many groups for which good values of the Charton steric factor is not known [17–23]. The Taft

Table 3. Variables, coefficient estimates, standard errors of estimates, and p values of the estimates for the β -signal prediction model

Variable	Coefficient	Standard error	p value
Intercept	126.537797	0.11	0.0001
F_1	-17.414998	2.66	0.0001
R_1	161.035505	5.62	0.0001
F_1F_1	46.617338	5.02	0.0001
F_1R_1	12.289252	4.66	0.0085
R_1R_1	40.675068	3.55	0.0001
R_1v_1	-387.548948	13.36	0.0001
R_1MR_1	3.036502	0.19	0.0001
v_1v_1	-23.102638	1.05	0.0001
F_2	26.377376	7.27	0.0003
R_2	-338.059053	20.81	0.0001
v_2	20.680575	1.41	0.0001
F_2F_2	-119.548130	18.09	0.0001
F_2R_2	-51.865701	7.02	0.0001
F_2v_2	93.790184	34.16	0.0061
F_2MR_2	-6.368708	1.03	0.0001
R_2R_2	-81.078698	5.66	0.0001
R_2v_2	971.799037	62.87	0.0001
F_2MR_2	-10.142096	0.65	0.0001
v_2v_2	56.137944	4.35	0.0001
F_3	-42.203092	4.62	0.0001
v_3	17.350969	2.13	0.0001
MR_3	-0.465757	0.14	0.0013
F_3F_3	-55.467863	7.95	0.0001
F_3R_3	-37.591915	4.90	0.0001
F_3v_3	132.587760	8.21	0.0001
F_3MR_3	-2.959668	0.43	0.0001
R_3v_3	72.537843	4.80	0.0001
R_3MR_3	-1.388971	0.21	0.0001
F_4	-1.773441	0.39	0.0001
R_4	-1.253745	0.39	0.0016
F_5	2.836571	0.50	0.0001
R_5	1.018114	0.42	0.0157
MR_5	-0.075999	0.02	0.0040
F_6	2.196643	0.47	0.0001
R_6	5.168925	0.38	0.0001
F_8	3.382608	0.57	0.0001
R_8	2.565087	0.42	0.0001
v_8	2.779425	0.92	0.0026
MR_8	-0.133938	0.05	0.0177

parameter, E_s , is known for a different set of groups [24], and it has been reported that a linear relationship exists between the two parameters [25]. This relationship is given by

$$E_s = -2.041480 v - 0.288578 \quad (r = 0.98) \quad (3)$$

We examined the two prediction equations given above with values of E_s used in place of v , and we found that although the coefficients changed in the equations, the predictive ability of the models was unaltered from those given above. As the v values are known for some groups and E_s for others, this refinement should lead to the use of larger databases in future studies of this type.

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Table 4. (in part). Compounds, observed and predicted ^{13}C NMR from positions 1–8. The *letters* in the encoding for a compound represent one of the substituents listed in Table 1. The encoding LE..... represents 1-acetyl-2-fluoronaphthalene, used as an example in the text. The *group numbers* listed in Table 1 are the numbers we have used for these groups in other papers. This is only part of Table 4. The complete Table 4 contains 394 compounds (3152 signals) and may be found in the Network Archives at <http://link.springer.de/journals/tea>

Compound	Position								Refs								
	1	2	3	4	5	6	7	8									
LE.....	121.6	123.7	156.8	157.0	114.5	115.1	131.7	134.1	127.0	127.8	124.4	126.0	127.0	128.0	123.5	123.3	37
L...E..	128.6	124.9	132.7	138.8	123.7	123.2	126.3	128.0	109.9	110.9	160.5	162.7	116.0	115.9	130.8	130.6	35
I.....	134.0	135.0	126.4	124.8	125.3	126.8	126.2	125.9	128.3	127.8	125.2	125.9	125.4	126.8	123.9	125.5	37
.I.....	126.7	126.9	135.2	134.8	127.9	128.4	127.2	127.6	127.5	127.8	124.8	125.8	125.7	126.5	127.4	127.0	37
AG.....	108.4	103.6	153.6	159.0	113.4	117.4	128.8	128.3	127.8	127.8	124.1	124.9	127.5	128.2	125.8	126.2	37
G...G...	155.3	156.1	104.6	107.6	125.1	126.2	114.3	117.3	155.3	156.1	104.6	107.6	125.1	126.2	114.3	117.3	37
P.....P	151.3	149.1	113.5	113.1	126.0	125.7	127.5	118.5	122.5	118.5	126.0	125.7	113.5	113.1	151.3	149.1	37
.C...E..	121.7	110.1	125.1	139.5	120.1	118.2	129.7	128.4	110.8	110.9	160.9	157.5	117.9	115.9	126.7	128.0	37
.H...I..	127.0	126.7	134.2	135.8	135.2	136.6	126.6	126.0	125.7	126.2	134.2	134.0	127.0	127.6	126.6	126.9	37
A.....	122.6	122.7	129.5	129.3	125.7	126.0	127.5	126.9	127.9	127.8	126.3	126.9	126.9	128.2	126.7	127.2	38
F...A...	151.1	150.8	109.1	107.6	129.3	129.5	113.4	115.2	127.0	127.2	127.8	128.2	126.0	126.8	121.3	122.2	38
AC.....	104.0	105.1	142.0	143.0	117.5	117.6	128.5	127.7	128.0	127.8	122.8	123.5	127.6	128.2	124.8	125.3	38
.C.....	107.9	110.1	146.9	140.3	119.1	118.2	129.4	128.6	128.3	127.8	122.2	123.1	126.7	126.5	126.2	125.9	41
.B....B.	125.7	125.7	132.8	132.1	127.0	126.9	129.2	129.3	129.2	129.3	127.0	126.9	126.9	132.1	125.7	125.7	43
.C.....	108.5	110.1	144.0	140.3	118.2	118.2	129.1	128.6	127.7	127.8	122.4	123.1	126.2	126.5	125.7	125.9	44
.L...G..	129.9	124.9	132.5	137.6	124.5	123.2	126.9	127.2	105.7	108.7	159.7	158.0	119.5	118.0	130.9	129.9	44
J....I..	146.9	150.0	122.1	122.1	124.2	125.1	134.2	130.7	127.7	126.9	137.6	136.3	131.8	131.7	122.1	123.6	48
.....G.	127.7	127.8	125.6	126.5	125.6	126.5	127.7	127.8	127.8	127.8	125.6	126.5	125.6	126.5	127.7	127.8	49
.G....G.	106.1	107.7	158.9	156.3	116.4	115.9	129.6	129.2	129.6	129.2	116.4	115.9	158.9	156.3	106.1	107.7	51
I...I..	126.6	126.9	134.3	134.0	128.1	128.4	127.0	126.9	126.6	126.9	134.3	134.0	128.1	128.4	127.0	126.9	36
BBB....	129.3	131.4	130.4	131.3	131.4	131.8	127.3	126.2	127.3	127.8	127.9	127.2	127.7	128.4	124.8	125.5	37
BBBBBBBB	128.7	128.1	135.0	133.2	135.0	133.2	128.7	128.1	128.7	128.1	135.0	133.2	135.0	133.2	128.7	128.1	37
JL...I..	148.2	149.1	130.0	130.3	128.2	127.0	127.1	130.5	126.5	126.9	136.8	135.5	130.8	131.7	121.1	122.9	48
G...GJ	157.5	154.7	107.0	109.9	126.5	122.5	140.2	144.8	127.3	128.9	118.4	119.6	150.4	153.6	135.0	125.5	51
JGJ...GJ	134.7	127.8	147.5	148.6	137.1	135.5	131.8	129.9	136.8	134.0	117.3	116.0	155.9	158.2	131.8	125.9	51

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