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# Molecular structure–property relationships for alkenes☆

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**Abstract**

Structure–property relationships were obtained for 11 physical and chemical properties (boiling points (bp), melting points (mp), molar refractions (MR), molar volumes (MV), heats of combustion (HCKJ), molar heats of vaporization (HVMOL), flashpoints (FLASHK), second virial coefficients (VIRC2), critical temperatures ($T_c$), critical pressures ($P_c$), and viscosities (VISC)) for a data set consisting of 162 C4–C9 monoalkenes. Both molecular connectivity indices and ad hoc descriptors were tested as structural descriptors, and both produced high-quality regression equations for most of the properties. As was observed in an earlier study of alkanes [J. Am. Chem. Soc. 110 (1988) 4186], mp were not well described by either descriptor set. For most properties, the mass/bulk of the molecule was found to be the most important structural feature determining the property, suggesting that dispersion forces play a dominant role in determining those properties influenced by intermolecular interactions. The amount of branching in the molecule and the nature of the double bond environment were also found to be influential features. 

*Keywords:* Structure–property relationships; Alkenes; Principal component analysis (PCA)

## 1. Introduction

One of the most fundamental ideas of chemistry is that the physical and chemical properties of a substance are determined, somehow, by its molecular structure — the term ‘structure’ taken here in its broadest sense to include both geometric and electronic aspects. Historically, the difficulty associated with this simple proposition has centered on how to implement it in practice, since finding appropriate mathematical terms to describe ‘molecular structure’ has not been easy. Such mathematical terms (‘descriptors’) are necessary if quantitative relationships are to be constructed between the structure of a compound and its properties. In principle, a full quantum mechanical treatment for a bulk property such as the boiling point (bp) should yield a solution to this conundrum, but in practice a full-blown, accurate quantum mechanical treatment of a sizable collection of molecules is presently out of the question. One turns, therefore, to simpler approaches. One such approach is to attempt to identify suitable quantum chemical descriptors obtained from studies of isolated molecules. This approach, although quite successful in some cases, has in many other cases produced only mixed results. A simpler, alternative approach is to employ topological descriptors, which fortunately often prove quite adequate to the task and, moreover, highly informative.

Several benefits can be derived from structure–property relationship studies. For example, unmeasured properties of related compounds can be estimated using the equations derived from a structure–property study. On a more fundamental level, a clearer understanding of the roles that specific structural features play in determining properties can be drawn from the equations. And once such an understanding is achieved, this information can be used to design hypothetical structures that might have desirable property values. Finally, the structure–property equations can serve as a useful check on the accuracy of property values already reported in the literature, some of which may be measured incorrectly or misreported.

In an earlier report [1] we applied topological descriptors in a study of eight physical properties of a set of normal and branched alkanes. In that study, it was found that of the topological descriptors examined, molecular connectivity indices [2,3] and ad hoc descriptors [1,4], were especially successful in yielding high-quality structure–property relationships. Good regression equations were obtained for seven of the physical properties of the alkanes (the melting points (mp), traditionally a subtle and difficult property to represent, were an exception). In this report, we employ these same descriptor types as structural measures for a study of the physical and chemical properties of a set of monoalkenes, where a new structural feature, the double bond, is introduced. Only

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a few previous QSPR studies have been devoted to the properties of this class of compounds [5–8], and these have generally been limited to single properties.

## 2. Methods

The properties examined in this study were: bp, molar refractions (MR), molar volumes (MV) at 20°C, heats of combustion (HCKJ), mp, molar heats of vaporization (HVMOL) at 25°C, flashpoints (FLASHK), second virial coefficients (VIRC2) at 25°C, critical temperatures ($T_c$), critical pressures ($P_c$), and viscosities (VISC) at 20°C. The property values were taken from reference sources [9–14]. MV were calculated as $M_w/d$, where $M_w$ is the molecular weight, and $d$ is the density (g/cm$^3$) at 20°C. MR were calculated using the Lorentz–Lorenz expression

$$\mathrm{MR} = \frac{(n_0^2 - 1)/(n_0^2 + 2)}{M_w/d}$$

where $n_0$ is the index of refraction.

The compounds examined and their shorthand abbreviations are listed in Appendix A. The property values for each compound are shown in Appendix B. The parameter values for each compound are shown in Appendix C.

Two types of parameters were used in this study: ad hoc descriptors [1,4] and molecular connectivity indices [2,3]. The ad hoc descriptors used were as follows: the number of carbon atoms (NC) represents the mass or bulk of the molecule. The square of the number of carbons (NCSC) and the square root (NCSR) account for non-linear aspects of the bulk dependence. The number of terminal methyl groups (TM) is a measure of the amount of branching in the molecule. The number of paths of length three carbon–carbon single bonds (P3S) is a steric index. The descriptor exterior double bonds (DBE) indicates whether the double bond is exterior or interior. The number of carbon atoms bonded to the double bond carbons (NCDB) measures the amount of crowding in the double bond environment. Several additional ad hoc indices were examined, but did not significantly improve the regression results.

Molecular connectivity indices were originally developed by Randic' [15], Kier and Hall [2,3]. The form of these descriptors is

$${}^m\chi_t^v$$

where $m$ is the order of the substructure, indicating the number of bonds, and t is the substructure type indicator. The substructure types included were path (p), cluster (c), path/cluster (pc), double bond (DB), and total (t) [1]. Only the valence (v) type indices, i.e. those which take explicit account of heteroatoms and multiple bonds, have been used in this study. The construction of these indices is described in detail in the alkane study [1] and elsewhere [2,3]. The molecular connectivity indices, used in this study, were calculated using Hall's MOLCONN2 software package [16]. Here, these indices are identified as

$$\mathrm{XV}(t)(m)(f)$$

where $f$ is the functional form (I = inverse, SQ = square, SR = square root). For example, XV1SR is the square root of the first order valence index, and XVPC4 is the fourth order pc index. Also included were the numbers of three-bond clusters (NXC3) and paths length of six bonds (NXP6). Altogether, 22 connectivity index terms were included in the initial screening.

Regression equations and other statistical measures were obtained using options in the SAS software package [17] on the Wright State University IBM 8083E computer. The final equations were selected on the basis of their standard errors (S.E.) and $F$-statistics. Principal component analysis (PCA) was used to determine the inherent dimensionality of the groups of properties. Orthogonal and oblique rotations did not significantly improve the results.

## 3. Results

### 3.1. Correlation analysis

The correlations among the properties examined are shown in Table 1. As can be seen, most of the properties

Table 1
Correlations among the properties examined

| | Bp | MR | MV | HCKJ | HVMOL | FLASHK | VIRC2 | $T_c$ | $P_c$ | VISC20 | Mp |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Bp | 1.000 | | | | | | | | | | |
| MR | 0.967 | 1.000 | | | | | | | | | |
| MV | 0.946 | 0.992 | 1.000 | | | | | | | | |
| HCKJ | 0.970 | 0.996 | 0.992 | 1.000 | | | | | | | |
| HVMOL | 0.993 | 0.921 | 0.903 | 0.938 | 1.000 | | | | | | |
| FLASHK | 0.933 | 0.905 | 0.844 | 0.897 | 0.878 | 1.000 | | | | | |
| VIRC2 | −0.960 | −0.981 | −0.969 | −0.976 | −0.974 | −0.975 | 1.000 | | | | |
| $T_c$ | 0.996 | 0.965 | 0.979 | 0.989 | 0.998 | 0.997 | −0.942 | 1.000 | | | |
| $P_c$ | −0.950 | −0.940 | −0.958 | −0.958 | −0.920 | −0.825 | 0.903 | −0.954 | 1.000 | | |
| VISC20 | 0.659 | 0.824 | 0.804 | 0.823 | 0.602 | 0.431 | −0.981 | 0.925 | −1.000 | 1.000 | |
| Mp | 0.664 | 0.640 | 0.614 | 0.525 | 0.482 | 0.518 | −0.543 | 0.607 | −0.467 | 0.844 | 1.000 |

Table 2
Multiple regression equation for the properties using ad hoc descriptors

| | |
|---|---|
| Bp (°C) | $-275.58(\pm3.51) + 139.31(\pm1.40) \times$ NCSR $+ 7.49(\pm0.36) \times$ NCDB $- 7.64(\pm0.26) \times$ TM $- 5.93(\pm0.62) \times$ DBE $+ 1.74(\pm0.19) \times$ P3S; $n = 162$, $r^2 = 0.9941$, S.E. $= 2.28$, $F = 5252$ |
| MR ($cm^3$/mol) | $20.65(\pm2.20) + 7.44(\pm0.35) \times$ NC $- 14.53(\pm1.76) \times$ NCSR $- 0.0862(\pm0.0130) \times$ P3S; $n = 156$, $r^2 = 0.9976$, S.E. $= 0.2224$, $F = 21114$ |
| MV ($cm^3$/mol) | $26.27(\pm0.66) + 17.33(\pm0.12) \times$ NC $- 1.99(\pm0.11) \times$ NCDB $- 1.27(\pm0.07) \times$ P3T $+ 0.87(\pm0.11) \times$ TM; $n = 156$, $r^2 = 0.9971$, S.E. $= 0.8547$, $F = 13105$ |
| HCKJ (kJ/mol) | $84.57(\pm2.89) + 659.83(\pm0.45) \times$ NC $- 8.83(\pm0.53) \times$ TM; $n = 65$, $r^2 = 1.0000$, S.E. $= 3.37$, $F = 1000000$ |
| Mp (°C) | $-169.58(\pm7.06) + 0.9947(\pm0.1508) \times$ NCSO; $n = 57$, $r^2 = 0.4416$, S.E. $= 17.43$, $F = 44$ |
| HVMOL (J/mol) | $-27094(\pm1150) + 24224(\pm490) \times$ NCSR $+ 1984(\pm192) \times$ NCDB $- 1972(\pm134) \times$ TM $- 1047(\pm237) \times$ DBE; $n = 34$, $r^2 = 0.9896$, S.E. $= 503$, $F = 690$ |
| FLASHK (K) | $22.08(\pm27.94) + 92.78(\pm11.25) \times$ NCSR; $n = 18$, $r^2 = 0.8096$, S.E. $= 5.81$, $F = 68$ |
| VIRC2 ($cm^3$/mol) | $3630(\pm597) + 111.5(\pm6.3) \times$ NCSO $+ 2427(\pm343) \times$ NCSR $- 68.5(\pm16.7) \times$ NCDB; $n = 14$, $r^2 = 0.9978$, S.E. $= 50.8$, $F = 1478$ |
| $T_c$ (°C) | $-63.73(\pm11.54) + 64.51(\pm3.90) \times$ NC·$2.30(\pm0.31) \times$ NCSO $- 10.42(\pm1.50) \times$ DBE; $n = 13$, $r^2 = 0.9981$, S.E. $= 2.45$, $F = 1607$ |
| $P_c$ (MPa) | $7.585(\pm0.319) - 1.789(\pm0.139) \times$ NCSR; $n = 12$, $r^2 = 0.9432$, S.E. $= 0.128$, $F = 166$ |
| VISC20 (cP) | $0.08661(\pm0.03813) + 0.00495(\pm0.00106) \times$ NCSO $+ 0.00884(\pm0.00167) \times$ TMSQ; $n = 6$, $r^2 = 0.9725$, S.E. $= 0.01843$, $F = 53$ |

are highly correlated with one another, with the exception of mp, which is poorly correlated with the other properties. VISC is another possible exception. The remaining nine properties all have correlation coefficients greater than 0.82, and the subset of bp, MR, MV, and HV all have correlations greater than 0.90.

### 3.2. Multiple regression analysis

Table 2 shows the most successful ad hoc descriptor models with their coefficients of determination ($r^2$), S.E., and $F$-values, and Table 3 shows these measures for the most successful molecular connectivity index models. Most of the

Table 3
Multiple regression equation for the properties using connectivity indices

| | |
|---|---|
| Bp (°C) | $15.04(\pm16.81) + 74.70(\pm6.08) \times$ XV1 $+ 307.40(\pm15.99) \times$ XVDB·$81.79(\pm5.36) \times$ XV0 $+ 28.49(\pm1.69) \times$ XVP3 $+ 51.20(\pm3.29) \times$ XVZ $+ 157.89(\pm16.49) \times$ XV1SR; $n = 162$, $r^2 = 0.9945$, S.E. $= 2.20$, $F = 46.80$ |
| MR ($cm^3$/mol) | $1.91(\pm0.57) + 8.87(\pm0.14) \times$ XV1 $+ 2.19(\pm0.04) \times$ XV2 $+ 14.00(\pm1.26) \times$ XVT; $n = 156$, $r^2 = 0.9973$, S.E. $= 0.2374$, $F = 18527$ |
| MV ($cm^3$/mol) | $7.79(\pm0.89) + 14.19(\pm0.36) \times$ XV1 $+ 14.21(\pm0.24) \times$ XV0 $+ 59.32(\pm1.58) \times$ XVDB $+ 0.14(\pm0.26) \times$ XVP3; $n = 156$, $r^2 = 0.9973$, S.E. $= 0.8340$, $F = 13766$ |
| HCKJ (kJ/mol) | $807.59(\pm10.34) + 1038.90(\pm3.81) \times$ XV1 $+ 308.07(12.51) \times$ XV2 $+ 103.80(\pm4.82) \times$ XVP3 $+ 35.22(\pm2.68) \times$ XVDB1; $n = 65$, $r^2 = 0.9998$, S.E. $= 6.44$, $F = 90708$ |
| Mp (°C) | $-414.50(\pm50.25) + 77.34(\pm12.22) \times$ XV1 $+ 491.59(\pm107.89) \times$ XVT; $n = 57$, $r^2 = 0.5510$, S.E. $= 15.77$, $F = 33$ |
| HVMOL (J/mol) | $-19604(\pm11.63) + 27409(\pm852) \times$ XV1SR $+ 2644(\pm246) \times$ XVDB1 $+ 1950(\pm282) \times$ NXP6; $n = 34$, $r^2 = 0.9884$, S.E. $= 523$, $F = 852$ |
| FLASHK (K) | $-113.57(\pm59.27) + 208.28(\pm30.67) \times$ XV1SR $+ 21291(\pm64.76) \times$ XVT; $n = 18$, $r^2 = 0.8982$, S.E. $= 44.5$, $F = 64$ |
| VIRC2 ($cm^3$/mol) | $1310.1(\pm145.7) + 405.7(\pm11.5) \times$ XV1SQ $+ 3421(\pm402) \times$ XVT $- 336(\pm46) \times$ XVPC4; $n = 14$, $r^2 = 0.9982$, S.E. $= 44.5$, $F = 1901$ |
| $T_c$ (°C) | $-440.18(\pm56.79) + 416.76(\pm35.72) \times$ XV1SR $+ 308.33(\pm50.29) \times$ XVT $+ 5.65(\pm1.22) \times$ XVT12; $n = 13$, $r^2 = 0.9974$, S.E. $= 2.90$, $F = 1151$ |
| $P_c$ (MPa) | $7.592(\pm0.336) + 1.051(\pm0.100) \times$ XV0 $+ 0.141(\pm0.025) \times$ XV1SQ $+ 4.135(\pm0.795) \times$ XVDB2; $n = 12$, $r^2 = 0.9878$, S.E. $= 0.066$, $F = 215$ |
| VISC20 (cP) | $0.2466(\pm0.0053) + 0.0454(\pm0.0023) \times$ NXC3 $+ 0.1034(\pm0.0108) \times$ NXP6; $n = 6$, $r^2 = 0.9028$, S.E. $= 0.0094$, $F = 208$ |

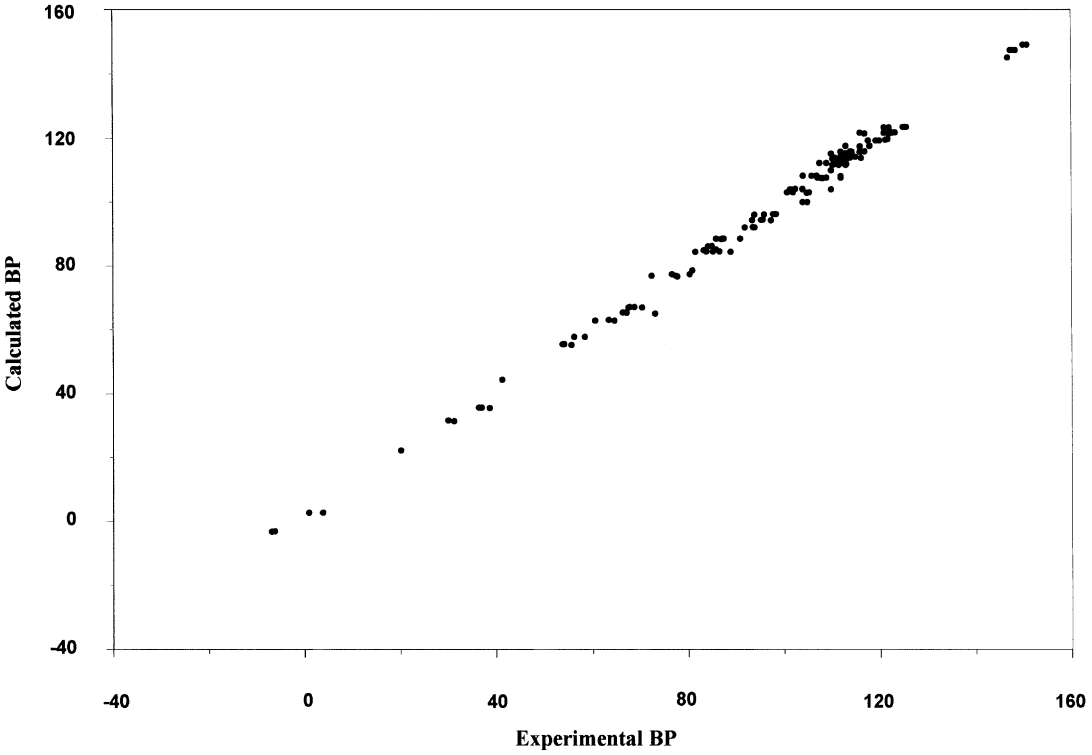


Fig. 1. Plot of calculated (ad hoc) boiling points vs. experimental boiling points.

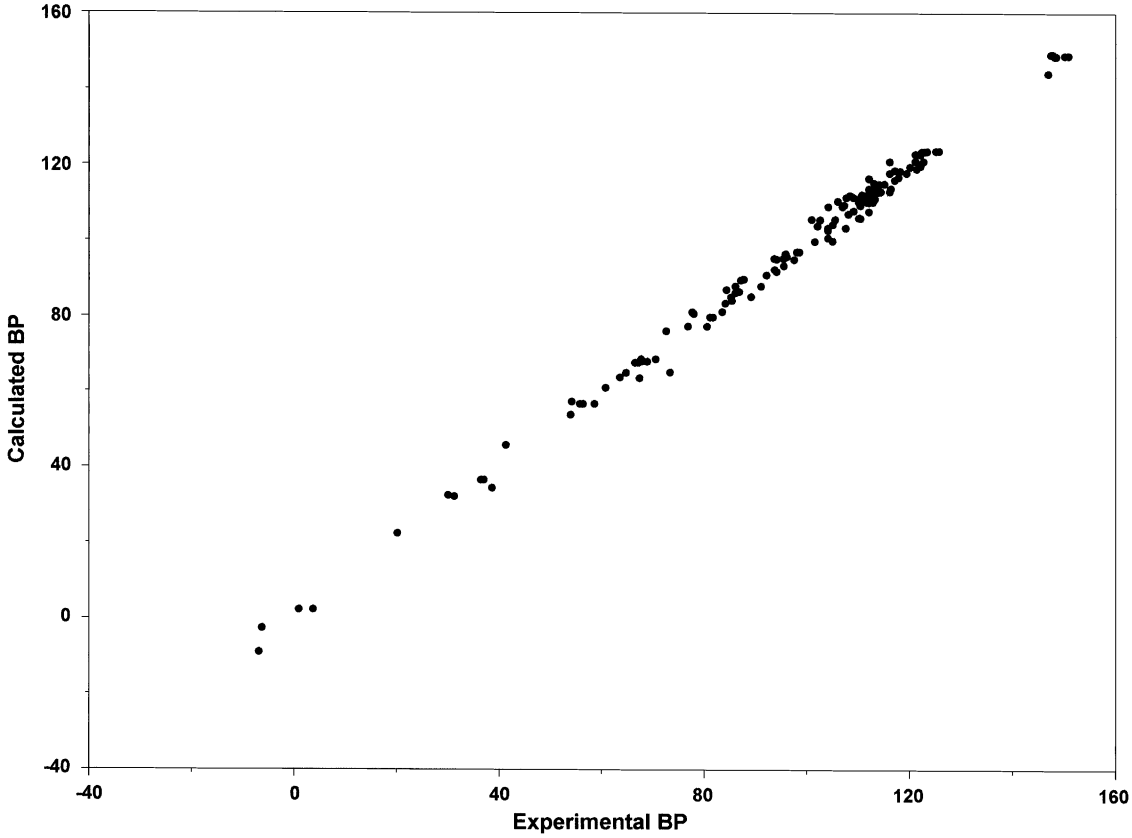


Fig. 2. Plot of calculated (molecular connectivity) boiling points vs. experimental boiling points.

Table 4
Results of the principal components analysis for the properties: eigenvalues with cumulative fractional variance reproduced

| Factor | Three properties (156 compounds) | Four properties (57 compounds) | Nine properties (11 compounds) |
|---|---|---|---|
| 1 | 2.937(0.979) | 3.446(0.862) | 7.632(0.848) |
| 2 | 0.058(0.998) | 0.501(0.987) | 1.079(0.968) |
| 3 | 0.005(1.000) | 0.047(0.999) | 0.148(0.984) |
| 4 | | 0.005(1.000) | 0.075(0.993) |
| 5 | | | 0.055(0.999) |

properties are reasonably well modeled by these two types of descriptors (Figs. 1 and 2), with the exception of the mp, which were not well modeled by either descriptor set. The FLASHK are less well modeled than most other properties, but this is not entirely unexpected since this property is difficult to measure and some reported values may be relatively inaccurate.

### 3.3. Factor analysis

Three factor analysis (PCA) studies were performed, focusing on differing sets of properties. These studies ranged from a 'compound intensive' study of just three properties (bp, MR, and MV), for which a large number of experimental values (156) were available, to a 'property intensive' study including nine properties, for which complete, matching data were available for only 11 compounds.

The results from the first factor analysis, using only bp, MR and MV, are shown in Table 4. As can be seen above, the three properties are highly correlated (Table 1) and a single factor dominates, accounting for 97.9% of the variation in these properties. As seen in Table 5, all three properties load strongly on the first factor. The data set is quite large ($n = 156$), and both low and high $M_w$ compounds are well represented.

Addition of mp to the analysis considerably reduced the size of the data set, to 57 compounds, but the set still retained a good sampling of both high and low $M_w$ compounds and remained large enough for reliable statistical calculations. The results are shown in Tables 4 and 5. As was seen in Table 1, the mp were not highly correlated with the other properties. The property set now appears to be represented by two factors (Table 4). The first factor accounts for 86.2% of the variance. Including the second factor, related to mp, brings this total to 98.7%. Reminiscent of the alkane study [1], bp, MR, and MV load heavily on the first factor, whereas mp loads strongly on the second factor.

Addition of the heat of combustion, the VIRC2, and the critical properties to the analysis markedly decreased the common compound population, and the population became strongly skewed toward the lower $M_w$ monoalkenes. The molar heat of vaporization was excluded to increase the number of compounds from 8 to 11. The results are shown in Tables 4 and 5. This analysis is included only for the sake

Table 5
PCA factor loadings for the physical properties

| Property | Factor | | |
|---|---|---|---|
| | 1 | 2 | 3 |
| Three properties | | | |
| Bp | 0.981 | 0.191 | 0.014 |
| MR | 0.997 | −0.054 | −0.055 |
| MV | 0.990 | −0.135 | 0.042 |
| Four properties | | | |
| Bp | 0.976 | −0.126 | −0.177 |
| MR | 0.982 | −0.174 | 0.056 |
| MV | 0.972 | −0.204 | 0.109 |
| Mp | 0.766 | 0.643 | 0.015 |
| Nine properties | | | |
| Bp | 0.968 | 0.163 | 0.173 |
| MR | 0.966 | −0.138 | −0.110 |
| MV | 0.982 | −0.093 | −0.096 |
| Mp | −0.062 | 0.993 | −0.100 |
| HCKJ | 0.998 | −0.004 | 0.017 |
| VIRC2 | −0.976 | −0.143 | −0.067 |
| $T_c$ | 0.971 | 0.106 | 0.187 |
| $P_c$ | −0.954 | 0.078 | 0.212 |
| VISC20 | 0.996 | −0.037 | −0.036 |

Table 6
Modeling of factor scores using structural descriptors

| Parameters | $r^2$ | S.E. | $F$ |
|---|---|---|---|
| Factor 1 | | | |
| NC | 0.9947 | 0.0726 | 29223 |
| NC, TMSQ | 0.9966 | 0.0585 | 22553 |
| NC, TMSQ, DBE | 0.9986 | 0.0382 | 35347 |
| XV1SR | 0.9684 | 0.1783 | 4720 |
| XV1SR, XV0 | 0.9936 | 0.0803 | 11929 |
| XV1SR, XV0, NXP6 | 0.9960 | 0.0638 | 12630 |
| Factor 2 | | | |
| NCDB | 0.0757 | 0.9701 | 5 |
| NCDB, NCSR | 0.1236 | 0.9533 | 4 |
| NCDB, NCSR, P3S | 0.2225 | 0.9063 | 5 |
| XVTSQ | 0.1564 | 0.9268 | 10 |
| XVTSQ, XV1SR | 0.3121 | 0.8446 | 12 |
| XVTSQ, XV1SR, XV1 | 0.3610 | 0.8217 | 10 |

of completeness, since its statistical significance is questionable. However, it is interesting to note that the first factor continued to dominate for most properties, accounting for 83.7% of the variance. Addition of the second factor brought this up to 97.0%, and the addition of a third factor brought this up to 99.8%.

In order to clarify, what the abstract factors represent, the factor scores were modeled using the ad hoc and connectivity descriptors. Factor 1 from the first analysis ($n = 156$) was employed to obtain a model for this factor, and Factor 2 was taken from the second analysis ($n = 57$) for the same purpose. The results are shown in Table 6. Factor 1 is clearly a bulk factor, depending on the leading descriptors, whereas Factor 2 was not well modeled by either of the descriptor sets.

## 4. Discussion

The regression equations presented in Tables 2 and 3 are generally of high-quality for properties other than the mp. Therefore, property values estimated on the basis of these equations, with the exception of mp, should be sufficiently accurate for many practical purposes.

The ad hoc descriptor equations in Table 2 show the relative influences of molecular mass/bulk (NC, NCSR and NCSQ), branching (TM), steric factors (P3S), and the double bond environment (DBE, NCDB) in determining the properties studied. As can be seen from the Table, the molecular mass/bulk clearly exerts the dominant influence for properties other than mp, suggesting that dispersion forces play a dominant role for those properties which depend on intermolecular forces. A similar conclusion was reached in the earlier alkane study [1,4]. This is a reasonable conclusion in the present case for bp, HVMOL, VIRC2, $T_c$, $P_c$, and VISC20. For MV the 'mass/bulk' dependence can be attributed directly to the larger volume of compounds with higher NC, as later modified by small corrections for branching and steric influences. Likewise, MR depends largely on the higher number of electrons in the larger compounds. For the two strictly "chemical" properties, the HCKJ and the flashpoints (FLASHK), the dependence on the mass/bulk dimension is more accurately attributed to the larger number of reacting bonds in the larger, higher NC compounds.

Branching, steric factors, and the double bond environment exert smaller influences on the properties, as demonstrated by the coefficients in the ad hoc regression equations. Molecular branching, represented by the number of TM sequesters interior parts of these compounds and reduces the extent of contact between neighboring molecules. The latter effect is reflected in the positive influence of TM on the MV. Because dispersion forces are strongly dependent on distance — the interaction energies fall as $1/r^6$, where $r$ is the separation — a decrease in the amount of close contact decreases the cohesive forces experienced by the compounds. Therefore, bp and HVKJ decrease as TM increases. Steric crowding, included here by the parameter P3S, leads to a small reduction in the MV, as reflected in the relatively small contributions to MV and MR from P3S. Whether the double bond is exterior or interior and the NSDB influence the accessibility of the double bond to its environment. When the double bond is exterior the bp, for example, is reduced on average by 6°C. Thus, DBE appear to exert a negative influence on the intermolecular forces. The NCDB exerts a positive influence on the intermolecular forces, possibly by effectively screening the effects of the double bond. Because of the above influences, those properties that depend on the strength of intermolecular forces, such as bp, HV, and $T_c$, show positive dependences on NC, NCSQ, NCSR, P3S, and NCDB, and negative dependences on TM and DBE.

The failure of both parameter sets to model the mp is not surprising, since this property was also not well modeled by these same topological parameters in our earlier study of the alkanes [1,4]. This illustrates the greater subtlety of the melting transition as compared to the boiling and critical transitions. The latter transitions involve a direct dependence on the operative intermolecular forces, and so directly reflect the strengths of these forces. The melting transition, in contrast, maintains a condensed phase and involves a partial disruption of intermolecular orientations. Melting, thus, depends on geometric and other factors that are not well addressed by the present topological parameters. This dependence on shape and entropic factors, as opposed to a simple intermolecular force dependence, is reflected in the mp strong loading on the second factor, rather than the first (mass/bulk related) factor, in the factor analysis. Dearden has recently given a comprehensive review of mp predictions [18].

Factor analysis for the monoalkenes shows that a single factor dominates for most properties. In the worst case examined (Analysis 3), Factor 1 still accounted for nearly 84% of the variance. Addition of a second factor in this case raised the variance accounted to 97%. Factor 1 is clearly related to the mass/bulk of the molecules. As can be seen, in Table 6 both the ad hoc and connectivity index mass/bulk dependent descriptors give a good account of this factor. Factor 2, however, is a different story. From the results in Table 5, it is obvious that Factor 2 is related to the mp, but this factor was not well modeled by either the ad hoc or connectivity index descriptors employed in this study. Because of this, it is difficult to determine exactly what structural features are crucial for this dimension.

## Acknowledgements

We thank Stephen Peterangelo for checking some of the regressions and preparing the figures.

## Appendix A. Compounds

| Observation no. | Name | Shorthand name |
|---|---|---|
| 1 | 1-Butene | 1N4 |
| 2 | *Cis*-2-butene | 2C4 |
| 3 | *Trans*-2-butene | 2T4 |
| 4 | 2-Methyl propene | 2M1N3 |
| 5 | 1-Pentene | 1N5 |
| 6 | *Cis*-2-pentene | 2C5 |
| 7 | *Trans*-2-pentene | 2T5 |
| 8 | 2-Methyl-1-butene | 2M1N4 |
| 9 | 3-Methyl-1-butene | 3M1N4 |
| 10 | 2-Methyl-2-butene | 2M2N4 |
| 11 | 1-Hexene | 1N6 |
| 12 | *Cis*-2-hexene | 2C6 |
| 13 | *Trans*-2-hexene | 2T6 |
| 14 | *Cis*-3-hexene | 3C6 |
| 15 | *Trans*-3-hexene | 3T6 |
| 16 | 2-Methyl-1-pentene | 2M1N5 |
| 17 | 3-Methyl-1-pentene | 3M1N5 |
| 18 | 4-Methyl-1-pentene | 4M1N5 |
| 19 | 2-Methyl-2-pentene | 2M2N5 |
| 20 | 3-Methyl-*cis*-2-pentene | 3M2C5 |
| 21 | 3-Methyl-*trans*-2-pentene | 3M2T5 |
| 22 | 4-Methyl-*cis*-2-pentene | 4M2C5 |
| 23 | 4-Methyl-*trans*-2-pentene | 4M2T5 |
| 24 | 2-Ethyl-1-butene | 2E1N4 |
| 25 | 2,3-Dimethyl-1-butene | 23M1N4 |
| 26 | 3,3-Dimethyl-1-butene | 33M1N4 |
| 27 | 2,3-Dimethyl-2-butene | 23M2N4 |
| 28 | 1-Heptene | 1N7 |
| 29 | *Cis*-2-heptene | 2C7 |
| 30 | *Trans*-2-heptene | 2T7 |
| 31 | *Cis*-3-heptene | 3C7 |
| 32 | *Trans*-3-heptene | 3T7 |
| 33 | 2-Methyl-1-hexene | 2M1N6 |
| 34 | 3-Methyl-1-hexene | 3M1N6 |
| 35 | 4-Methyl-1-hexene | 4M1N6 |
| 36 | 5-Methyl-1-hexene | 5M1N6 |
| 37 | 2-Methyl-2-hexene | 2M2N6 |
| 38 | 3-Methyl-*cis*-2-hexene | 3M2C6 |
| 39 | 3-Methyl-*trans*-2-hexene | 3M2T6 |
| 40 | 4-Methyl-*cis*-2-hexene | 4M2C6 |
| 41 | 4-Methyl-*trans*-2-hexene | 4M2T6 |
| 42 | 5-Methyl-*cis*-2-hexene | 5M2C6 |
| 43 | 5-Methyl-*trans*-2-hexene | 5M2T6 |
| 44 | 2-Methyl-*cis*-3-hexene | 2M3C6 |
| 45 | 2-Methyl-*trans*-3-hexene | 2M3T6 |
| 46 | 3-Methyl-*cis*-3-hexene | 3M3C6 |
| 47 | 3-Methyl-*trans*-3-hexene | 3M3T6 |
| 48 | 2-Ethyl-1-pentene | 2E1N5 |
| 49 | 3-Ethyl-1-pentene | 3E1N5 |
| 50 | 2,3-Dimethyl-1-pentene | 23M1N5 |
| 51 | 2,4-Dimethyl-1-pentene | 24M1N5 |
| 52 | 3,3-Dimethyl-1-pentene | 33M1N5 |
| 53 | 3,4-Dimethyl-1-pentene | 34M1N5 |
| 54 | 4,4-Dimethyl-1-pentene | 44M1N5 |

Appendix A (*Continued*)

| Observation no. | Name | Shorthand name |
|---|---|---|
| 55 | 3-Ethyl-2-pentene | 3E2N5 |
| 56 | 2,3-Dimethyl-2-pentene | 23M2N5 |
| 57 | 2,4-Dimethyl-2-pentene | 24M2N5 |
| 58 | 3,4-Dimethyl-*cis*-2-pentene | 34M2C5 |
| 59 | 3,4-Dimethyl-*trans*-2-pentene | 34M2T5 |
| 60 | 4,4-Dimethyl-*cis*-2-pentene | 44M2C5 |
| 61 | 4, 4-Dimethyl-*trans*-2-pentene | 44M2T5 |
| 62 | 2-Ethyl-3-methyl-1-butene | 2E3M1N4 |
| 63 | 2,3,3-Trimethyl-1-butene | 233M1N4 |
| 64 | 1-Octene | 1N8 |
| 65 | *Cis*-2-octene | 2C8 |
| 66 | *Trans*-2-octene | 2T8 |
| 67 | *Cis*-3-octene | 3C8 |
| 68 | *Trans*-3-octene | 3T8 |
| 69 | *Cis*-4-octene | 4C8 |
| 70 | *Trans*-4-octene | 4T8 |
| 71 | 2-Methyl-1-heptene | 2M1N7 |
| 72 | 3-Methyl-1-heptene | 3M1N7 |
| 73 | 4-Methyl-1-heptene | 4M1N7 |
| 74 | 5-Methyl-1-heptene | 5M1N7 |
| 75 | 6-Methyl-1-heptene | 6M1N7 |
| 76 | 2-Methyl-2-heptene | 2M2N7 |
| 77 | 3-Methyl-*cis*-2-heptene | 3M2C7 |
| 78 | 3-Methyl-*trans*-2-heptene | 3M2T7 |
| 79 | 4-Methyl-*cis*-2-heptene | 4M2C7 |
| 80 | 4-Methyl-*trans*-2-heptene | 4M2T7 |
| 81 | 5-Methyl-*cis*-2-heptene | 5M2C7 |
| 82 | 5-Methyl-*trans*-2-heptene | 5M2T7 |
| 83 | 6-Methyl-*cis*-2-heptene | 6M2C7 |
| 84 | 6-Methyl-*trans*-2-heptene | 6M2T7 |
| 85 | 2-Methyl-*cis*-3-heptene | 2M3C7 |
| 86 | 2-Methyl-*trans*-3-heptene | 2M3T7 |
| 87 | 3-Methyl-*cis*-3-heptene | 3M3C7 |
| 88 | 3-Methyl-*trans*-3-heptene | 3M3T7 |
| 89 | 4-Methyl-*cis*-3-heptene | 4M3C7 |
| 90 | 4-Methyl-*trans*-3-heptene | 4M3T7 |
| 91 | 5-Methyl-*cis*-3-heptene | 5M3C7 |
| 92 | 5-Methyl-*trans*-3-heptene | 5M3T7 |
| 93 | 6-Methyl-*cis*-3-heptene | 6M3C7 |
| 94 | 6-Methyl-*trans*-3-heptene | 6M3T7 |
| 95 | 2-Ethyl-1-hexene | 2E1N6 |
| 96 | 3-Ethyl-1-hexene | 3E1N6 |
| 97 | 4-Ethyl-1-hexene | 4E1N6 |
| 98 | 2,3-Dimethyl-1-hexene | 23M1N6 |
| 99 | 2,4-Dimethyl-1-hexene | 24M1N6 |
| 100 | 2,5-Dimethyl-1-hexene | 25M1N6 |
| 101 | 3,3-Dimethyl-1-hexene | 33M1N6 |
| 102 | 3,4-Dimethyl-1-hexene | 34M1N6 |
| 103 | 3,5-Dimethyl-1-hexene | 35M1N6 |
| 104 | 4,4-Dimethyl-1-hexene | 44M1N6 |
| 105 | 4,5-Dimethyl-1-hexene | 45M1N6 |
| 106 | 5,5-Dimethyl-1-hexene | 55M1N6 |
| 107 | 3-Ethyl-*cis*-2-hexene | 3E2C6 |
| 108 | 3-Ethyl-*trans*-2-hexene | 3E2T6 |

Appendix A (*Continued*)

| Observation no. | Name | Shorthand name |
|---|---|---|
| 109 | 4-Ethyl-*cis*-2-hexene | 4E2C6 |
| 110 | 4-Ethyl-*trans*-2-hexene | 4E2T6 |
| 111 | 2,3-Dimethyl-2-hexene | 23M2N6 |
| 112 | 2,4-Dimethyl-2-hexene | 24M2N6 |
| 113 | 2,5-Dimethyl-2-hexene | 25M2N6 |
| 114 | 3,4-Dimethyl-*cis*-2-hexene | 34M2C6 |
| 115 | 3,4-Dimethyl-*trans*-2-hexene | 34M2T6 |
| 116 | 3,5-Dimethyl-*cis*-2-hexene | 35M2C6 |
| 117 | 3,5-Dimethyl-*trans*-2-hexene | 35M2T6 |
| 118 | 4,4-Dimethyl-*cis*-2-hexene | 44M2C6 |
| 119 | 4,4-Dimethyl-*trans*-2-hexene | 44M2T6 |
| 120 | 4,5-Dimethyl-*cis*-2-hexene | 45M2C6 |
| 121 | 4,5-Dimethyl-*trans*-2-hexene | 45M2T6 |
| 122 | 5,5-Dimethyl-*cis*-2-hexene | 55M2C6 |
| 123 | 5,5-Dimethyl-*trans*-2-hexene | 55M2T6 |
| 124 | 3-Ethy1-3-hexene | 3E3N6 |
| 125 | 2,2-Dimethyl-*cis*-3-hexene | 22M3C6 |
| 126 | 2,2-Dimethyl-*trans*-3-hexene | 22M3T6 |
| 127 | 2,3-Dimethyl-*cis*-3-hexene | 23M3C6 |
| 128 | 2,3-Dimethyl-*trans*-3-hexene | 23M3T6 |
| 129 | 2,4-Dimethyl-*cis*-3-hexene | 24M3C6 |
| 130 | 2,4-Dimethyl-*trans*-3-hexene | 24M3T6 |
| 131 | 2,5-Dimethyl-*cis*-3-hexene | 25M3C6 |
| 132 | 2,5-Dimethyl-*trans*-3-hexene | 25M3T6 |
| 133 | 3,4-Dimethyl-*cis*-3-hexene | 34M3C6 |
| 134 | 3,4-Dimethyl-*trans*-3-hexene | 34M3T6 |
| 135 | 2-*n*-Propyl-1-pentene | 2NP1N5 |
| 136 | 2-Isopropyl-1-pentene | 21P1N5 |
| 137 | 2-Ethyl-3-methyl-1-pentene | 2E3M1N5 |
| 138 | 2-Ethyl-4-methyl-1-pentene | 2E4M1N5 |
| 139 | 3-Ethyl-2-methyl-1-pentene | 3E2M1N5 |
| 140 | 3-Ethyl-3-methyl-1-pentene | 3E3M1N5 |
| 141 | 3-Ethyl-4-methyl-1-pentene | 3E4M1N5 |
| 142 | 2,3,3-Trimethyl-1-pentene | 233M1N5 |
| 143 | 2,3,4-trimethyl-1-pentene | 234M1N5 |
| 144 | 2,4,4-Trimethyl-1-pentene | 244M1N5 |
| 145 | 3,3,4-Trimethyl-1-pentene | 334M1N5 |
| 146 | 3,4,4-Trimethyl-1-pentene | 344M1N5 |
| 147 | 3-Ethyl-2-methyl-2-pentene | 3E2M2N5 |
| 148 | 3-Ethyl-4-methyl-*cis*-2-pentene | 3E4M2C5 |
| 149 | 3-Ethyl-4-methyl-*trans*-2-pentene | 3E4M2T5 |
| 150 | 2,3,4-Trimethyl-2-pentene | 234M2N5 |
| 151 | 2,4,4-Trimethyl-2-pentene | 244M2N5 |
| 152 | 3,4,4-Trimethyl-*cis*-2-pentene | 344M2C5 |
| 153 | 3,4,4-Trimethyl-*trans*-2-pentene | 344M2T5 |
| 154 | 2-Isopropyl-3-methyl-1-butene | 21P3M1N4 |
| 155 | 2-Ethyl-3,3-dimethyl-1-butene | 2E33M1N4 |
| 156 | 1-Nonene | 1N9 |
| 157 | *Cis*-2-nonene | 2C9 |
| 158 | *Trans*-2-nonene | 2T9 |
| 159 | *Cis*-3-nonene | 3C9 |
| 160 | *Trans*-3-nonene | 3T9 |
| 161 | *Cis*-4-nonene | 4C9 |
| 162 | *Trans*-4-nonene | 4T9 |

## Appendix B. Property values

| Observation no. | Shorthand name | bp | mp | MR | MV | HCKJ | HVMOL | FLASHK | VIRC2 | $T_c$ | $P_c$ | VISC20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1N4 | −6.260 | −185.35 | 22.6628 | 94.277 | 2716.8 | 20204 | – | −649.7 | 146.450 | 4.023 | – |
| 2 | 2C4 | 3.720 | −138.91 | 20.5879 | 90.301 | 2710.0 | 21963 | – | −712.9 | 162.430 | 4.205 | – |
| 3 | 2T4 | 0.880 | −105.55 | 20.7281 | 92.857 | 2706.4 | 21483 | – | −700.1 | 155.480 | 4.104 | – |
| 4 | 2M1N3 | −6.9000 | −140.35 | 22.6311 | 94.419 | 2700.2 | 20101 | – | −647.7 | 144.760 | 4.000 | – |
| 5 | 1N5 | 29.968 | −165.22 | 24.8543 | 109.43 | 3375.4 | 25501 | – | −1092.7 | 191.630 | 3.526 | 0.2390 |
| 6 | 2C5 | 36.942 | −151.39 | 24.9524 | 106.971 | 3370.0 | 26885 | – | −1150.3 | 201.790 | 3.695 | – |
| 7 | 2T5 | 36.353 | −140.24 | 25.0200 | 108.192 | 3365.4 | – | 228.15 | −1140.0 | 201.850 | 3.648 | – |
| 8 | 2M1N4 | 31.163 | −137.56 | 24.8474 | 107.826 | 3361.6 | – | – | −1111.0 | 191.850 | 3.505 | – |
| 9 | 3M1N4 | 20.061 | −168.49 | 24.9416 | 111.814 | 3368.9 | – | – | −973.9 | 191.850 | 3.435 | – |
| 10 | 2M2N4 | 38.568 | −133.77 | 24.9521 | 105.889 | 3355.7 | 27090 | 228.15 | −1264.0 | 197.240 | 3.380 | – |
| 11 | 1N6 | 63.485 | −139.82 | 29.4915 | 125.014 | 4034.1 | 30587 | 247.15 | −1729.0 | 230.800 | 3.140 | 0.2600 |
| 12 | 2C6 | 68.840 | −141.13 | 29.5309 | 122.462 | 4023.8 | 33744 | – | – | – | – | – |
| 13 | 2T6 | 67.870 | −132.97 | 29.6684 | 124.133 | 4022.2 | 32136 | 253.15 | – | – | – | – |
| 14 | 3C6 | 66.440 | −137.82 | 29.6605 | 123.777 | 4028.5 | 31724 | – | – | – | – | – |
| 15 | 3T6 | 67.080 | −113.43 | 29.7493 | 124.287 | 4021.7 | 32072 | 261.15 | – | – | – | – |
| 16 | 2M1N6 | 60.700 | −135.72 | 29.4759 | 123.782 | 4016.8 | 31042 | 247.15 | – | – | – | – |
| 17 | 3M1N5 | 54.140 | −153.00 | 29.4946 | 126.086 | 4026.1 | 29262 | 245.15 | – | – | – | – |
| 18 | 4M1N5 | 53.880 | −153.63 | 29.5548 | 126.798 | 4024.9 | 29376 | 242.15 | – | – | – | 0.2883 |
| 19 | 2M2N5 | 67.290 | −135.07 | 29.7378 | 122.587 | 4007.3 | 32088 | 250.15 | – | – | – | – |
| 20 | 3M2C5 | 70.450 | −138.44 | 29.5488 | 122.213 | 4013.9 | 31812 | – | – | – | – | – |
| 21 | 4M2C5 | 67.630 | −134.84 | 29.5498 | 121.437 | 4013.0 | 32536 | – | – | – | – | – |
| 22 | 4M2C5 | 56.300 | −134.43 | 29.6707 | 125.760 | 4018.7 | 30096 | 245.15 | – | – | – | – |
| 23 | 4M2T5 | 58.550 | −140.81 | 29.7533 | 125.865 | 4014.7 | 30550 | – | – | – | – | – |
| 24 | 2E1N4 | 64.660 | −131.53 | 29.3700 | 122.040 | 4020.2 | 31614 | – | – | – | – | 0.2885 |
| 25 | 23M1N4 | 55.670 | −157.27 | 29.4338 | 124.106 | 4011.2 | 29800 | 255.15 | – | – | – | – |
| 26 | 33M1N4 | 41.240 | −115.20 | 29.5814 | 128.856 | 4015.4 | 27449 | 245.15 | – | – | – | – |
| 27 | 23M2N4 | 73.210 | −74.28 | 29.5944 | 118.848 | 4007.3 | 32476 | 257.15 | −1929.0 | – | – | – |
| 28 | 1N7 | 93.643 | −119.03 | 34.1347 | 140.868 | 4692.6 | 35484 | 272.15 | −2810.0 | 264.145 | – | 0.3500 |
| 29 | 2C7 | 98.500 | – | 34.1730 | 138.852 | 4686.5 | – | – | – | – | – | – |
| 30 | 2T7 | 97.950 | −109.48 | 34.2812 | 140.020 | 4682.3 | – | 272.15 | – | – | – | – |
| 31 | 3C7 | 95.750 | – | 34.3076 | 139.701 | 4686.5 | – | – | – | – | – | – |
| 32 | 3T7 | 95.670 | −136.63 | 34.4259 | 140.642 | 4682.3 | – | – | – | – | – | – |
| 33 | 2M1N6 | 92.000 | −102.84 | 34.1237 | 139.681 | 4678.0 | – | 267.15 | – | – | – | – |
| 34 | 3M1N6 | 84.000 | – | 34.1588 | 142.005 | 4688.7 | – | 267.15 | – | – | – | – |
| 35 | 4M1N6 | 86.730 | −141.45 | 34.0754 | 140.561 | 4688.7 | – | – | – | – | – | – |
| 36 | 5M1N6 | 85.310 | – | 34.1444 | 141.882 | 4686.0 | – | – | – | – | – | – |
| 37 | 2M2N6 | 95.410 | −130.35 | 34.3978 | 138.656 | 4672.2 | – | – | – | – | – | – |
| 38 | 3M2C6 | 94.000 | – | 34.1783 | 137.183 | 4674.9 | – | – | – | – | – | – |

Appendix B (*Continued*)

| Observation no. | Shorthand name | bp | mp | MR | MV | HCKJ | HVMOL | FLASHK | VIRC2 | $T_c$ | $P_c$ | VISC20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 39 | 3M2T6 | 94.000 | – | 34.1889 | 137.452 | 4674.9 | – | – | – | – | – | – |
| 40 | 4N2C6 | 87.370 | – | 34.2220 | 140.360 | 4682.0 | – | – | – | – | – | – |
| 41 | 4M2T6 | 87.600 | −126.50 | 34.3471 | 140.904 | 4677.8 | – | – | – | – | – | – |
| 42 | 5M2C6 | 91.000 | – | 34.2048 | 139.860 | 4679.3 | – | – | – | – | – | – |
| 43 | 5M2T6 | 86.000 | – | 34.4113 | 141.759 | 4675.1 | – | – | – | – | – | – |
| 44 | 2M3C6 | 86.000 | – | 34.3721 | 141.473 | 4679.3 | – | – | – | – | – | – |
| 45 | 2M3T6 | 86.000 | – | 34.5228 | 142.375 | 4675.1 | – | – | – | – | – | – |
| 46 | 3M3C6 | 95.350 | – | 34.3169 | 137.728 | 4674.9 | – | – | – | – | – | – |
| 47 | 3M3T6 | 93.550 | – | 34.3448 | 138.353 | 4674.9 | – | – | – | – | – | – |
| 48 | 2E1N5 | 94.000 | – | 33.9890 | 138.675 | 4680.7 | – | – | – | – | – | – |
| 49 | 3E1N5 | 85.130 | −127.40 | 34.0617 | 141.066 | 4691.3 | – | – | – | – | – | – |
| 50 | 23M1N5 | 84.260 | −134.80 | 33.9975 | 139.226 | 4673.8 | – | – | – | – | – | – |
| 51 | 24M1N5 | 81.640 | −123.80 | 34.1793 | 141.452 | 4670.9 | 33344 | – | – | – | – | – |
| 52 | 33M1N5 | 77.540 | −134.30 | 34.0085 | 140.783 | 4679.4 | – | – | – | – | – | – |
| 53 | 34M1N5 | 81.000 | – | 34.0542 | 140.722 | 4681.7 | – | – | – | – | – | – |
| 54 | 44M1N5 | 72.490 | −136.60 | 34.2349 | 143.859 | 4674.7 | 31598 | – | – | – | – | – |
| 55 | 3E2N5 | 96.010 | – | 34.1144 | 136.288 | 4677.5 | – | – | – | – | – | – |
| 56 | 23M2N5 | 97.46 | −118.30 | 34.2218 | 134.921 | 4667.1 | – | – | – | – | – | – |
| 57 | 24M2N5 | 83.44 | – | 34.5314 | 141.285 | 4665.1 | 34418 | – | – | – | – | – |
| 58 | 34M2C5 | 87.00 | – | 34.1229 | 137.606 | 4667.9 | – | – | – | – | – | – |
| 59 | 34M2T5 | 87.00 | – | 34.1452 | 136.992 | 4667.9 | – | – | – | – | – | – |
| 60 | 44M2C5 | 80.42 | −135.46 | 34.2255 | 140.374 | 4667.9 | 32973 | – | – | – | – | – |
| 61 | 44M2T5 | 76.75 | −115.23 | 34.4054 | 142.530 | 4663.9 | 33187 | – | – | – | – | – |
| 62 | 2E3M1N4 | 89.00 | – | 33.9649 | 138.523 | 4673.7 | 34634 | – | – | – | – | – |
| 63 | 233M1N4 | 77.87 | −109.85 | 33.9878 | 139.332 | 4668.2 | 32485 | 256.15 | – | – | – | 0.475 |
| 64 | 1N8 | 121.26 | −101.74 | 38.7781 | 156.952 | 5351.1 | 41224 | – | −3948 | – | – | – |
| 65 | 2C8 | 125.64 | −100.20 | 38.7944 | 154.919 | – | – | – | – | – | – | – |
| 66 | 2T8 | 125.00 | −87.70 | 38.8827 | 155.866 | – | – | – | – | – | – | – |
| 67 | 3C8 | 122.90 | – | 38.8482 | 155.828 | – | – | – | – | – | – | – |
| 68 | 3T8 | 123.30 | −110.00 | 39.0883 | 156.890 | – | – | – | – | – | – | – |
| 69 | 4C8 | 122.54 | −118.70 | 38.9447 | 155.585 | – | – | – | – | – | | – |
| 70 | 4T8 | 122.25 | −93.81 | 39.0817 | 157.132 | – | – | – | – | – | | – |
| 71 | 2M1N7 | 119.30 | −90.00 | 38.7759 | 155.736 | – | – | – | – | – | | – |
| 72 | 3M1N7 | 111.00 | – | 38.7649 | 157.817 | – | – | – | – | – | – | – |
| 73 | 4M1N7 | 112.80 | – | 38.7739 | 156.497 | – | – | – | – | – | – | – |
| 74 | 5M1N7 | 113.30 | – | 38.7564 | 156.628 | – | – | – | – | – | – | – |
| 75 | 6M1N7 | 113.20 | – | 38.7944 | 157.596 | – | – | – | – | – | – | – |
| 76 | 2M2N7 | 122.60 | – | 38.9693 | 154.962 | – | – | – | – | – | – | – |
| 77 | 3M2C7 | 122.00 | – | 38.8702 | 153.920 | – | – | – | – | – | – | – |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 78 | 3M2T7 | 122.00 | – | 38.8702 | 153.920 | – | – | – | – | – | – | – |
| 79 | 4M2C7 | 114.00 | – | 38.8281 | 156.715 | – | – | – | – | – | – | – |
| 80 | 4M2T7 | 114.00 | – | 38.8281 | 156.715 | – | – | – | – | – | – | – |
| 81 | 5M2C7 | 118.00 | – | 38.7819 | 155.198 | – | – | – | – | – | – | – |
| 82 | 5M2T7 | 118.00 | – | 38.7819 | 155.198 | – | – | – | – | – | – | – |
| 83 | 6M2C7 | 117.00 | – | 38.8860 | 156.279 | – | – | – | – | – | – | – |
| 84 | 6M2T7 | 117.00 | – | 38.8860 | 156.279 | – | – | – | – | – | – | – |
| 85 | 2M3C7 | 112.00 | – | 39.1241 | 158.935 | – | – | – | – | – | – | – |
| 86 | 2M3T7 | 112.00 | – | 39.1241 | 158.935 | – | – | – | – | – | – | – |
| 87 | 3M3C7 | 121.00 | – | 38.8421 | 154.132 | – | – | – | – | – | – | – |
| 88 | 3M3T7 | 121.00 | – | 38.8421 | 154.132 | – | – | – | – | – | – | – |
| 89 | 4M3C7 | 122.00 | – | 38.9209 | 154.770 | – | – | – | – | – | – | – |
| 90 | 4M3T7 | 122.00 | – | 38.9209 | 154.770 | – | – | – | – | – | – | – |
| 91 | 5M3C7 | 112.00 | – | 38.9914 | 157.374 | – | – | – | – | – | – | – |
| 92 | 5M3T7 | 112.00 | – | 38.9914 | 157.374 | – | – | – | – | – | – | – |
| 93 | 6M3C7 | 115.00 | – | 38.9914 | 157.374 | – | – | – | – | – | – | – |
| 94 | 6M3T7 | 115.00 | – | 38.9914 | 157.374 | – | – | – | – | – | – | – |
| 95 | 2E1N6 | 120.00 | – | 38.7076 | 154.344 | – | – | – | – | – | – | – |
| 96 | 3E1N6 | 110.30 | – | 38.6317 | 156.934 | – | – | – | – | – | – | – |
| 97 | 4E1N6 | 113.00 | – | 38.4575 | 154.556 | – | – | – | – | – | – | – |
| 98 | 23M1N6 | 110.50 | – | 38.7028 | 155.542 | – | – | – | – | – | – | – |
| 99 | 24M1N6 | 111.20 | – | 38.6952 | 155.844 | – | – | – | – | – | – | – |
| 100 | 25M1N6 | 111.60 | – | 38.8047 | 156.453 | – | – | – | – | – | – | – |
| 101 | 33M1N6 | 104.00 | – | 38.6858 | 157.154 | – | – | – | – | – | – | – |
| 102 | 34M1N6 | 112.00 | – | 38.6461 | 154.983 | – | – | – | – | – | – | – |
| 103 | 35M1N6 | 104.00 | – | 38.7599 | 158.486 | – | – | – | – | – | – | – |
| 104 | 44M1N6 | 107.20 | – | 38.6397 | 155.888 | – | – | – | – | – | – | – |
| 105 | 45M1N6 | 109.00 | – | 38.5155 | 154.132 | – | – | – | – | – | – | – |
| 106 | 55M1N6 | 102.50 | – | 38.7813 | 158.262 | – | – | – | – | – | – | – |
| 107 | 3E2C6 | 121.00 | – | 38.8499 | 152.250 | – | – | – | – | – | – | – |
| 108 | 3E2T6 | 121.00 | – | 38.8499 | 152.250 | – | – | – | – | – | – | – |
| 109 | 4E2C6 | 113.00 | – | 38.5106 | 154.770 | – | – | – | – | – | – | – |
| 110 | 4E2T6 | 113.00 | – | 38.5106 | 154.770 | – | – | – | – | – | – | – |
| 111 | 23M2N6 | 121.770 | −115.10 | 38.8737 | 151.469 | – | – | – | – | – | – | – |
| 112 | 24M2N6 | 110.600 | – | 38.6916 | 155.564 | – | – | – | – | – | – | – |
| 113 | 25M2N6 | 112.200 | – | 38.9435 | 155.844 | – | – | – | – | – | – | – |
| 114 | 34M2C6 | 116.000 | – | 38.3677 | 152.250 | – | – | – | – | – | – | – |
| 115 | 34M2T6 | 116.000 | – | 38.3677 | 152.250 | – | – | – | – | – | – | – |
| 116 | 35M2C6 | 112.000 | – | 38.8390 | 154.770 | – | – | – | – | – | – | – |
| 117 | 35M2T6 | 112.000 | – | 38.8390 | 154.770 | – | – | – | – | – | – | – |
| 118 | 44M2C6 | 106.000 | – | 38.7531 | 155.413 | – | – | – | – | – | – | – |
| 119 | 44M2T6 | 106.000 | – | 38.7531 | 155.413 | – | – | – | – | – | – | – |
| 120 | 45M2C6 | 110.000 | – | 38.5928 | 154.770 | – | – | – | – | – | – | – |
| 121 | 45M2T6 | 110.000 | – | 38.5928 | 154.770 | – | – | – | – | – | – | – |
| 122 | 55M2C6 | 106.900 | – | 38.8875 | 156.518 | – | – | – | – | – | – | – |

Appendix B (*Continued*)

| Observation no. | Shorthand name | bp | mp | MR | MV | HCKJ | HVMOL | FLASHK | VIRC2 | $T_c$ | $P_c$ | VISC20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 123 | 55M2T6 | 104.100 | – | 38.9639 | 158.800 | – | – | – | – | – | – | – |
| 124 | 3E3N6 | 116.000 | – | 38.7888 | 153.920 | – | – | – | – | – | – | – |
| 125 | 22M3C6 | 105.430 | −137.35 | 38.9940 | 157.419 | – | – | – | – | – | – | – |
| 126 | 22M3T6 | 100.850 | – | 39.1814 | 159.409 | – | – | – | – | – | – | – |
| 127 | 23M3C6 | 114.000 | – | 38.6789 | 154.132 | – | – | – | – | – | – | – |
| 128 | 23M3T6 | 114.000 | – | 38.6789 | 154.132 | – | – | – | – | – | – | – |
| 129 | 24M3C6 | 109.000 | – | 39.0628 | 156.322 | – | – | – | – | – | – | – |
| 130 | 24M3T6 | 107.600 | – | 39.1266 | 157.044 | – | – | – | – | – | – | – |
| 131 | 25M3C6 | 102.000 | – | 38.8195 | 158.039 | – | – | – | – | – | – | – |
| 132 | 25M3T6 | 102.000 | – | 38.8195 | 158.039 | – | – | – | – | – | – | – |
| 133 | 34M3C6 | 122.000 | – | 38.8034 | 150.212 | – | – | – | – | – | – | – |
| 134 | 34M3T6 | 122.000 | – | 38.8034 | 150.212 | – | – | – | – | – | – | – |
| 135 | 2NP1N5 | 117.700 | – | 38.6954 | 154.983 | – | – | – | – | – | – | – |
| 136 | 2IP1N5 | 113.000 | – | 38.6749 | 154.770 | – | – | – | – | – | – | – |
| 137 | 2E3M1N5 | 112.500 | – | 38.4790 | 153.920 | – | – | – | – | – | – | – |
| 138 | 2E4M1N5 | 110.300 | – | 38.6806 | 155.953 | – | – | – | – | – | – | – |
| 139 | 3E2M1N5 | 110.000 | – | 38.4915 | 153.710 | – | – | – | – | – | – | – |
| 140 | 3E3M1N5 | 112.000 | – | 38.7091 | 153.604 | – | – | – | – | – | – | – |
| 141 | 3E4M1N5 | 107.500 | – | 38.5875 | 155.844 | – | – | – | – | – | – | – |
| 142 | 233M1N5 | 108.310 | −69.00 | 38.4132 | 152.622 | – | – | – | – | – | – | – |
| 143 | 234M1N5 | 108.000 | | 38.5443 | 153.920 | – | – | – | – | – | – | – |
| 144 | 244M1N5 | 101.440 | −93.48 | 38.7654 | 156.934 | – | – | – | – | – | – | – |
| 145 | 334M1N5 | 105.000 | – | 38.4953 | 153.920 | – | – | – | – | – | – | – |
| 146 | 344M1N5 | 104.000 | – | 38.8320 | 156.061 | – | – | – | – | – | – | – |
| 147 | 3E2M2N5 | 117.000 | – | 38.8007 | 151.838 | – | – | – | – | – | – | – |
| 148 | 3E4M2C5 | 116.000 | – | 38.7447 | 151.838 | – | – | – | – | – | – | – |
| 149 | 3E4M2T5 | 114.300 | – | 38.7141 | 152.664 | – | – | – | – | – | – | – |
| 150 | 234M2N5 | 116.260 | −133.30 | 38.7933 | 150.939 | – | – | – | – | – | – | – |
| 151 | 244M2N5 | 104.910 | −106.33 | 39.0111 | 155.456 | – | 37224 | – | – | – | – | – |
| 152 | 344M2C5 | 112.000 | – | 38.6647 | 151.838 | – | – | – | – | – | – | – |
| 153 | 344M2T5 | 112.000 | – | 38.6647 | 151.838 | – | – | – | – | – | – | – |
| 154 | 2IP3M1N4 | 104.000 | – | 38.3813 | 155.413 | – | – | – | – | – | – | – |
| 155 | 2E33N1N4 | 110.000 | – | 38.6707 | 154.132 | – | – | – | – | – | – | – |
| 156 | 1N9 | 146.868 | −81.37 | 43.4462 | 173.232 | 6010.1 | – | – | – | 320.1 | 2.33 | – |
| 157 | 2C9 | 150.823 | – | – | – | – | – | – | – | – | – | – |
| 158 | 2T9 | 150.073 | – | – | – | – | – | – | – | – | – | – |
| 159 | 3C9 | 148.440 | – | – | – | – | – | – | – | – | – | – |
| 160 | 3T9 | 148.179 | – | – | – | – | – | – | – | – | – | – |
| 161 | 4C9 | 147.420 | – | – | – | | – | – | – | – | – | – |
| 162 | 4T9 | 147.773 | – | – | – | – | – | – | – | – | – | – |

## Appendix C. Parameter values

| Observation no. | Shorthand name | NC | TM | P3S | P3T | NCDB | DBE | XV0 | XV1 | XV2 | XVP3 | XVDB | XVT | XVPC4 | NXP6 | NXC3 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1N4 | 4 | 1 | 0 | 1 | 1 | 1 | 2.9916 | 1.5236 | 0.6969 | 0.2887 | 0.408248 | 0.288675 | 0.0000 | 0 | 0 |
| 2 | 2C4 | 4 | 2 | 0 | 1 | 2 | 0 | 3.1547 | 1.4880 | 0.6667 | 0.3333 | 0.333333 | 0.333333 | 0.0000 | 0 | 0 |
| 3 | 2T4 | 4 | 2 | 0 | 1 | 2 | 0 | 3.1547 | 1.4880 | 0.6667 | 0.3333 | 0.333333 | 0333333 | 0.0000 | 0 | 0 |
| 4 | 2M1N3 | 4 | 2 | 0 | 0 | 2 | 1 | 3.2071 | 1.3536 | 1.2071 | 0.0000 | 0.353553 | 0.353553 | 0.0000 | 0 | 1 |
| 5 | 1N5 | 5 | 1 | 1 | 2 | 1 | 1 | 3.6987 | 2.0236 | 1.0774 | 0.4928 | 0.408248 | 0.204124 | 0.0000 | 0 | 0 |
| 6 | 2C5 | 5 | 2 | 0 | 2 | 2 | 0 | 3.8618 | 2.0260 | 0.9773 | 0.4714 | 0.333333 | 0.235702 | 0.0000 | 0 | 0 |
| 7 | 2T5 | 5 | 2 | 0 | 2 | 2 | 0 | 3.8618 | 2.0260 | 0.9773 | 0.4714 | 0.333333 | 0.235702 | 0.0000 | 0 | 0 |
| 8 | 2M1N4 | 5 | 2 | 1 | 2 | 2 | 1 | 3.9142 | 1.9142 | 1.3107 | 0.6036 | 0.353553 | 0.250000 | 0.2500 | 0 | 1 |
| 9 | 3M1N4 | 5 | 2 | 0 | 2 | 1 | 1 | 3.8618 | 1.8963 | 1.4797 | 0.4714 | 0.408248 | 0.235702 | 0.2357 | 0 | 1 |
| 10 | 2M2N4 | 5 | 3 | 0 | 2 | 3 | 0 | 4.0774 | 1.8660 | 1.3660 | 0.5774 | 0.288675 | 0.288675 | 0.2887 | 0 | 1 |
| 11 | 1N6 | 6 | 1 | 2 | 3 | 1 | 1 | 4.4058 | 2.5236 | 1.4309 | 0.7618 | 0.408248 | 0.144338 | 0.0000 | 0 | 0 |
| 12 | 2C6 | 6 | 2 | 1 | 3 | 2 | 0 | 4.5689 | 2.5260 | 1.3577 | 0.6910 | 0.333333 | 0.166667 | 0.0000 | 0 | 0 |
| 13 | 2T6 | 6 | 2 | 1 | 3 | 2 | 0 | 4.5689 | 2.5260 | 1.3577 | 0.6910 | 0.333333 | 0.166667 | 0.0000 | 0 | 0 |
| 14 | 3C6 | 6 | 2 | 0 | 3 | 2 | 0 | 4.5689 | 2.5640 | 1.2879 | 0.6381 | 0.333333 | 0.166667 | 0.0000 | 0 | 0 |
| 15 | 3T6 | 6 | 2 | 0 | 3 | 2 | 0 | 4.5689 | 2.5640 | 1.2879 | 0.6381 | 0.333333 | 0.166667 | 0.0000 | 0 | 0 |
| 16 | 2M1N5 | 6 | 2 | 2 | 3 | 2 | 1 | 4.6213 | 2.4142 | 1.7071 | 0.6768 | 0.353553 | 0.176777 | 0.1768 | 0 | 1 |
| 17 | 3M1N5 | 6 | 2 | 2 | 3 | 1 | 1 | 4.5689 | 2.4343 | 1.6212 | 1.0463 | 0.408248 | 0.166667 | 0.4024 | 0 | 1 |
| 18 | 4M1N5 | 6 | 2 | 2 | 3 | 1 | 1 | 4.5689 | 2.3794 | 1.9182 | 0.6381 | 0.408248 | 0.166667 | 0.2357 | 0 | 1 |
| 19 | 2M2N5 | 6 | 3 | 0 | 3 | 3 | 0 | 4.7845 | 2.4040 | 1.6897 | 0.6124 | 0.288675 | 0.204124 | 0.2041 | 0 | 1 |
| 20 | 3M2C5 | 6 | 3 | 1 | 4 | 3 | 0 | 4.7845 | 2.4267 | 1.4886 | 1.0505 | 0.288675 | 0.204124 | 0.4082 | 0 | 1 |
| 21 | 3M2T5 | 6 | 3 | 1 | 4 | 3 | 0 | 4.7845 | 2.4267 | 1.4886 | 1.0505 | 0.288675 | 0.204124 | 0.4082 | 0 | 1 |
| 22 | 4M2C5 | 6 | 3 | 0 | 3 | 2 | 0 | 4.7321 | 2.3987 | 1.7698 | 0.5774 | 0.333333 | 0.192450 | 0.1925 | 0 | 1 |
| 23 | 4M2T5 | 6 | 3 | 0 | 3 | 2 | 0 | 4.7321 | 2.3987 | 1.7698 | 0.5774 | 0.333333 | 0.192450 | 0.1925 | 0 | 1 |
| 24 | 2E1N4 | 6 | 2 | 2 | 4 | 2 | 1 | 4.6213 | 2.4749 | 1.4571 | 1.0000 | 0.353553 | 0.176777 | 0.3536 | 0 | 1 |
| 25 | 23M1N4 | 6 | 3 | 2 | 4 | 2 | 1 | 4.7845 | 2.2969 | 2.0011 | 0.9856 | 0.353553 | 0.204124 | 0.9010 | 0 | 2 |
| 26 | 33M1N4 | 6 | 3 | 0 | 3 | 1 | 1 | 4.7845 | 2.1969 | 2.5701 | 0.6124 | 0.408248 | 0.204124 | 0.4082 | 0 | 4 |
| 27 | 23M2N4 | 6 | 4 | 0 | 4 | 4 | 0 | 5.0000 | 2.2500 | 2.0000 | 1.0000 | 0.250000 | 0.250000 | 1.0000 | 0 | 2 |
| 28 | 1N7 | 7 | 1 | 3 | 4 | 1 | 1 | 5.1129 | 3.0236 | 1.7845 | 1.0118 | 0.408248 | 0.102062 | 0.0000 | 1 | 0 |
| 29 | 2C7 | 7 | 2 | 2 | 4 | 2 | 0 | 5.2760 | 3.0260 | 1.7113 | 0.9600 | 0.333333 | 0.117851 | 0.0000 | 1 | 0 |
| 30 | 2T7 | 7 | 2 | 2 | 4 | 2 | 0 | 5.2760 | 3.0260 | 1.7113 | 0.9600 | 0.333333 | 0.117851 | 0.0000 | 1 | 0 |
| 31 | 3C7 | 7 | 2 | 1 | 4 | 2 | 0 | 5.2760 | 3.0640 | 1.6683 | 0.8577 | 0.333333 | 0.117851 | 0.0000 | 1 | 0 |
| 32 | 3T7 | 7 | 2 | 1 | 4 | 2 | 0 | 5.2760 | 3.0640 | 1.6683 | 0.8577 | 0.333333 | 0.117851 | 0.0000 | 1 | 0 |
| 33 | 2M1N6 | 7 | 2 | 3 | 4 | 2 | 1 | 5.3284 | 2.9142 | 2.0607 | 0.9571 | 0.353553 | 0.125000 | 0.1768 | 0 | 1 |
| 34 | 3M1N6 | 7 | 2 | 3 | 5 | 1 | 1 | 5.2760 | 2.9343 | 2.0017 | 1.1464 | 0.408248 | 0.117851 | 0.3333 | 0 | 1 |
| 35 | 4M1N6 | 7 | 2 | 3 | 5 | 1 | 1 | 5.2760 | 2.9175 | 2.0378 | 1.2660 | 0.408248 | 0.117851 | 0.4553 | 0 | 1 |
| 36 | 5M1N6 | 7 | 2 | 3 | 4 | 1 | 1 | 5.2760 | 2.8794 | 2.2599 | 0.9481 | 0.408248 | 0.117851 | 0.2887 | 0 | 1 |
| 37 | 2M2N6 | 7 | 3 | 1 | 4 | 3 | 0 | 5.4916 | 2.9040 | 2.0701 | 0.8413 | 0.288675 | 0.144338 | 0.2041 | 0 | 1 |
| 38 | 3M2C6 | 7 | 3 | 2 | 5 | 3 | 0 | 5.4916 | 2.9267 | 1.8850 | 1.1371 | 0.288675 | 0.144338 | 0.3485 | 0 | 1 |
| 39 | 3M2T6 | 7 | 3 | 2 | 5 | 3 | 0 | 5.4916 | 2.9267 | 1.8850 | 1.1371 | 0.288675 | 0.144338 | 0.3485 | 0 | 1 |
| 40 | 4M2C6 | 7 | 3 | 2 | 5 | 2 | 0 | 5.4392 | 2.9367 | 1.9113 | 1.1649 | 0.333333 | 0.136083 | 0.3718 | 0 | 1 |

Appendix C (*Continued*)

| Observation no. | Shorthand name | NC | TM | P3S | P3T | NCDB | DBE | XV0 | XV1 | XV2 | XVP3 | XVDB | XVT | XVPC4 | NXP6 | NXC3 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 41 | 4M2T6 | 7 | 3 | 2 | 5 | 2 | 0 | 5.4392 | 2.9367 | 1.9113 | 1.1649 | 0.333333 | 0.136083 | 0.3718 | 0 | 1 |
| 42 | 5M2C6 | 7 | 3 | 2 | 4 | 2 | 0 | 5.4392 | 2.8819 | 2.1986 | 0.8432 | 0.333333 | 0.136083 | 0.2357 | 0 | 1 |
| 43 | 5M2T6 | 7 | 3 | 2 | 4 | 2 | 0 | 5.4392 | 2.8819 | 2.1986 | 0.8432 | 0.333333 | 0.136083 | 0.2357 | 0 | 1 |
| 44 | 2M3C6 | 7 | 3 | 0 | 4 | 2 | 0 | 5.4392 | 2.9367 | 2.0804 | 0.7587 | 0.333333 | 0.136083 | 0.1925 | 0 | 1 |
| 45 | 2M3T6 | 7 | 3 | 0 | 4 | 2 | 0 | 5.4392 | 2.9367 | 2.0804 | 0.7567 | 0.333333 | 0.136083 | 0.1925 | 0 | 1 |
| 46 | 3M3C6 | 7 | 3 | 1 | 5 | 3 | 0 | 5.4916 | 2.9647 | 1.8123 | 1.1103 | 0.288675 | 0.144338 | 0.3485 | 0 | 1 |
| 47 | 3M3T6 | 7 | 3 | 1 | 5 | 3 | 0 | 5.4916 | 2.9647 | 1.8123 | 1.1103 | 0.288675 | 0.144338 | 0.3485 | 0 | 1 |
| 48 | 2E1N5 | 7 | 2 | 3 | 5 | 2 | 1 | 5.3284 | 2.9749 | 1.8536 | 1.1036 | 0.353553 | 0.125000 | 0.3018 | 0 | 1 |
| 49 | 3E1N5 | 7 | 2 | 4 | 6 | 1 | 1 | 5.2760 | 2.9723 | 1.8123 | 1.3821 | 0.408248 | 0.117851 | 0.4512 | 0 | 1 |
| 50 | 23M1N5 | 7 | 3 | 4 | 6 | 2 | 1 | 5.4916 | 2.8349 | 2.1556 | 1.4536 | 0.353553 | 0.144338 | 0.9010 | 0 | 2 |
| 51 | 24M1N5 | 7 | 3 | 3 | 4 | 2 | 1 | 5.4916 | 2.7701 | 2.5551 | 0.7567 | 0.353553 | 0.144338 | 0.3485 | 0 | 2 |
| 52 | 33M1N5 | 7 | 3 | 3 | 5 | 1 | 1 | 5.4916 | 2.7576 | 2.5463 | 1.4638 | 0.408248 | 0.144338 | 0.6969 | 0 | 4 |
| 53 | 34M1N5 | 7 | 3 | 4 | 6 | 1 | 1 | 5.4392 | 2.8070 | 2.3388 | 1.4234 | 0.408248 | 0.138083 | 1.0468 | 0 | 2 |
| 54 | 44M1N5 | 7 | 3 | 3 | 4 | 1 | 1 | 5.4916 | 2.6700 | 3.0535 | 0.7567 | 0.408248 | 0.144338 | 0.4082 | 0 | 4 |
| 55 | 3E2N5 | 7 | 3 | 2 | 6 | 3 | 0 | 5.4916 | 2.9873 | 1.6540 | 1.3165 | 0.288675 | 0.144338 | 0.4330 | 0 | 1 |
| 56 | 23M2N5 | 7 | 4 | 1 | 6 | 4 | 0 | 5.7071 | 2.8107 | 2.1339 | 1.3839 | 0.250000 | 0.176777 | 0.9571 | 0 | 2 |
| 57 | 24M2N5 | 7 | 4 | 0 | 4 | 3 | 0 | 5.6547 | 2.7767 | 2.4880 | 0.6667 | 0.288675 | 0.166667 | 0.3333 | 0 | 2 |
| 58 | 34M2C5 | 7 | 4 | 2 | 6 | 3 | 0 | 5.6547 | 2.8094 | 2.1874 | 1.3660 | 0.288675 | 0.166667 | 0.9553 | 0 | 2 |
| 59 | 34M2T5 | 7 | 4 | 2 | 6 | 3 | 0 | 5.6547 | 2.8094 | 2.1874 | 1.3660 | 0.288675 | 0.166667 | 0.9553 | 0 | 2 |
| 60 | 44M2C5 | 7 | 4 | 0 | 4 | 2 | 0 | 5.6547 | 2.6994 | 2.8660 | 0.6667 | 0.333333 | 0.166667 | 0.3333 | 0 | 4 |
| 61 | 44M2T5 | 7 | 4 | 0 | 4 | 2 | 0 | 5.6547 | 2.6994 | 2.8660 | 0.6667 | 0.333333 | 0.166667 | 0.3333 | 0 | 4 |
| 62 | 2E3M1N4 | 7 | 3 | 3 | 6 | 2 | 1 | 5.4916 | 2.8576 | 2.1665 | 1.2706 | 0.353553 | 0.144338 | 0.8413 | 0 | 2 |
| 63 | 233M1N4 | 7 | 4 | 3 | 6 | 2 | 1 | 5.7071 | 2.6036 | 3.0303 | 1.2803 | 0.353553 | 0.176777 | 1.3839 | 0 | 5 |
| 64 | 1N8 | 8 | 1 | 4 | 5 | 1 | 1 | 5.8200 | 3.5236 | 2.1380 | 1.2618 | 0.408248 | 0.072169 | 0.0000 | 2 | 0 |
| 65 | 2C8 | 8 | 2 | 3 | 5 | 2 | 0 | 5.9831 | 3.5260 | 2.0648 | 1.2100 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 66 | 2T8 | 8 | 2 | 3 | 5 | 2 | 0 | 5.9831 | 3.5260 | 2.0648 | 1.2100 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 67 | 3C8 | 8 | 2 | 2 | 5 | 2 | 0 | 5.9831 | 3.5640 | 2.0219 | 1.1267 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 68 | 3T8 | 8 | 2 | 2 | 5 | 2 | 0 | 5.9831 | 3.5640 | 2.0219 | 1.1267 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 69 | 4C8 | 8 | 2 | 2 | 5 | 2 | 0 | 5.9831 | 3.5640 | 2.0488 | 1.0774 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 70 | 4T8 | 8 | 2 | 2 | 5 | 2 | 0 | 5.9831 | 3.5640 | 2.0488 | 1.0774 | 0.333333 | 0.083333 | 0.0000 | 2 | 0 |
| 71 | 2M1N7 | 8 | 2 | 4 | 5 | 2 | 1 | 6.0355 | 3.4142 | 2.4142 | 1.2071 | 0.353553 | 0.088388 | 0.1768 | 2 | 1 |
| 72 | 3M1N7 | 8 | 2 | 4 | 6 | 1 | 1 | 5.9831 | 3.4343 | 2.3552 | 1.4154 | 0.408248 | 0.083333 | 0.3333 | 1 | 1 |
| 73 | 4M1N7 | 8 | 2 | 5 | 6 | 1 | 1 | 5.9831 | 3.4175 | 2.4182 | 1.3505 | 0.408248 | 0.083333 | 0.3708 | 1 | 1 |
| 74 | 5M1N7 | 8 | 2 | 5 | 6 | 1 | 1 | 5.9831 | 3.4175 | 2.3794 | 1.5605 | 0.408248 | 0.083333 | 0.4928 | 1 | 1 |
| 75 | 6M1N7 | 8 | 2 | 4 | 5 | 1 | 1 | 5.9831 | 3.3794 | 2.6134 | 1.1897 | 0.408248 | 0.083333 | 0.2887 | 2 | 1 |
| 76 | 2M2N7 | 8 | 3 | 2 | 5 | 3 | 0 | 6.1987 | 3.4040 | 2.4237 | 1.1103 | 0.288675 | 0.102062 | 0.2041 | 2 | 1 |
| 77 | 3M2C7 | 8 | 3 | 3 | 6 | 3 | 0 | 6.1987 | 3.4267 | 2.2386 | 1.4175 | 0.288675 | 0.102062 | 0.3485 | 1 | 1 |
| 78 | 3M2T7 | 8 | 3 | 3 | 6 | 3 | 0 | 6.1987 | 3.4267 | 2.2386 | 1.4175 | 0.288675 | 0.102062 | 0.3485 | 1 | 1 |
| 79 | 4M2C7 | 8 | 3 | 3 | 6 | 2 | 0 | 6.1463 | 3.4367 | 2.2917 | 1.2650 | 0.333333 | 0.096225 | 0.3027 | 1 | 1 |
| 80 | 4M2T7 | 8 | 3 | 3 | 6 | 2 | 0 | 6.1463 | 3.4367 | 2.2917 | 1.2650 | 0.333333 | 0.096225 | 0.3027 | 1 | 1 |

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 81 | 5M2C7 | 8 | 3 | 4 | 6 | 2 | 0 | 6.1463 | 3.4199 | 2.3182 | 1.4711 | 0.333333 | 0.096225 | 0.4553 | 1 | 1 |
| 82 | 5M2T7 | 8 | 3 | 4 | 6 | 2 | 0 | 6.1463 | 3.4199 | 2.3182 | 1.4711 | 0.333333 | 0.096225 | 0.4553 | 1 | 1 |
| 83 | 6M2C7 | 8 | 3 | 3 | 5 | 2 | 0 | 6.1463 | 3.3819 | 2.5402 | 1.1464 | 0.333333 | 0.096225 | 0.2887 | 2 | 1 |
| 84 | 6M2T7 | 8 | 3 | 3 | 5 | 2 | 0 | 6.1463 | 3.3819 | 2.5402 | 1.1464 | 0.333333 | 0.096225 | 0.2887 | 2 | 1 |
| 85 | 2M3C7 | 8 | 3 | 1 | 5 | 2 | 0 | 6.1463 | 3.4367 | 2.4608 | 0.9763 | 0.333333 | 0.096225 | 0.1925 | 2 | 1 |
| 86 | 2M3T7 | 8 | 3 | 1 | 5 | 2 | 0 | 6.1463 | 3.4367 | 2.4608 | 0.9763 | 0.333333 | 0.096225 | 0.1925 | 2 | 1 |
| 87 | 3M3C7 | 8 | 3 | 2 | 6 | 3 | 0 | 6.1987 | 3.4647 | 2.1927 | 1.3392 | 0.288675 | 0.102062 | 0.3485 | 1 | 1 |
| 88 | 3M3T7 | 8 | 3 | 2 | 6 | 3 | 0 | 6.1987 | 3.4647 | 2.1927 | 1.3392 | 0.288675 | 0.102062 | 0.3485 | 1 | 1 |
| 89 | 4M3C7 | 8 | 3 | 2 | 6 | 3 | 0 | 6.1987 | 3.4647 | 2.2087 | 1.1969 | 0.288675 | 0.102062 | 0.2887 | 1 | 1 |
| 90 | 4M3T7 | 8 | 3 | 2 | 6 | 3 | 0 | 6.1987 | 3.4647 | 2.2087 | 1.1969 | 0.288675 | 0.102062 | 0.2887 | 1 | 1 |
| 91 | 5M3C7 | 8 | 3 | 2 | 6 | 2 | 0 | 6.1463 | 3.4747 | 2.2219 | 1.3443 | 0.333333 | 0.096225 | 0.3718 | 1 | 1 |
| 92 | 5M3T7 | 8 | 3 | 2 | 6 | 2 | 0 | 6.1463 | 3.4747 | 2.2219 | 1.3443 | 0.333333 | 0.096225 | 0.3718 | 1 | 1 |
| 93 | 6M3C7 | 8 | 3 | 2 | 5 | 2 | 0 | 6.1463 | 3.4199 | 2.5092 | 1.0099 | 0.333333 | 0.096225 | 0.2357 | 2 | 1 |
| 94 | 6M3T7 | 8 | 3 | 2 | 5 | 2 | 0 | 6.1463 | 3.4199 | 2.5092 | 1.0099 | 0.333333 | 0.096225 | 0.2357 | 2 | 1 |
| 95 | 2E1N6 | 8 | 2 | 4 | 6 | 2 | 1 | 6.0355 | 3.4749 | 2.2071 | 1.3839 | 0.353553 | 0.088388 | 0.3018 | 1 | 1 |
| 96 | 3E1N6 | 8 | 2 | 5 | 7 | 1 | 1 | 5.9831 | 3.4723 | 2.1927 | 1.5172 | 0.408248 | 0.083333 | 0.4024 | 0 | 1 |
| 97 | 4E1N6 | 8 | 2 | 6 | 7 | 1 | 1 | 5.9831 | 3.4555 | 2.2069 | 1.8547 | 0.408248 | 0.083333 | 0.5261 | 0 | 1 |
| 98 | 23M1N6 | 8 | 3 | 5 | 7 | 2 | 1 | 6.1987 | 3.3349 | 2.5361 | 1.5629 | 0.353553 | 0.1020682 | 0.8413 | 0 | 2 |
| 99 | 24M1N6 | 8 | 3 | 5 | 6 | 2 | 1 | 6.1987 | 3.3081 | 2.6747 | 1.3938 | 0.353553 | 0.102062 | 0.5774 | 0 | 2 |
| 100 | 25M1N6 | 8 | 3 | 4 | 5 | 2 | 1 | 6.1987 | 3.2701 | 2.8896 | 1.1485 | 0.353553 | 0.102062 | 0.4655 | 0 | 2 |
| 101 | 33M1N6 | 8 | 3 | 4 | 7 | 1 | 1 | 6.1987 | 3.2576 | 2.9427 | 1.4469 | 0.408248 | 0.102062 | 0.5774 | 0 | 4 |
| 102 | 34M1N6 | 8 | 3 | 6 | 8 | 1 | 1 | 6.1463 | 3.3450 | 2.4804 | 1.9133 | 0.408248 | 0.096225 | 1.0721 | 0 | 2 |
| 103 | 35M1N6 | 8 | 3 | 4 | 6 | 1 | 1 | 6.1463 | 3.2901 | 2.8425 | 1.2456 | 0.408248 | 0.096225 | 0.5385 | 0 | 2 |
| 104 | 44M1N6 | 8 | 3 | 6 | 7 | 1 | 1 | 6.1987 | 3.2307 | 3.0106 | 1.6540 | 0.408248 | 0.102062 | 0.7887 | 0 | 4 |
| 105 | 45M1N6 | 8 | 3 | 6 | 7 | 1 | 1 | 6.1463 | 3.2901 | 2.7457 | 1.6765 | 0.408248 | 0.096225 | 1.1765 | 0 | 2 |
| 106 | 55M1N6 | 8 | 3 | 4 | 5 | 1 | 1 | 6.1987 | 3.1701 | 3.3880 | 1.0985 | 0.408248 | 0.102062 | 0.5000 | 0 | 4 |
| 107 | 3E2C6 | 8 | 3 | 3 | 7 | 3 | 0 | 6.1987 | 3.4873 | 2.0505 | 1.4335 | 0.288675 | 0.102062 | 0.3907 | 0 | 1 |
| 108 | 3E2T6 | 8 | 3 | 3 | 7 | 3 | 0 | 6.1987 | 3.4873 | 2.0505 | 1.4335 | 0.288675 | 0.102082 | 0.3907 | 0 | 1 |
| 109 | 4E2C6 | 8 | 3 | 4 | 7 | 2 | 0 | 6.1463 | 3.4747 | 2.1024 | 1.5134 | 0.333333 | 0.096225 | 0.4296 | 0 | 1 |
| 110 | 4E2T6 | 8 | 3 | 4 | 7 | 2 | 0 | 6.1463 | 3.4747 | 2.1024 | 1.5134 | 0.333333 | 0.096225 | 0.4296 | 0 | 1 |
| 111 | 23M2N6 | 8 | 4 | 1 | 7 | 4 | 0 | 6.4142 | 3.3107 | 2.5303 | 1.4786 | 0.250000 | 0.125000 | 0.9053 | 0 | 2 |
| 112 | 24M2N6 | 8 | 4 | 2 | 6 | 3 | 0 | 6.3618 | 3.3147 | 2.6295 | 1.2618 | 0.288675 | 0.117851 | 0.5202 | 0 | 2 |
| 113 | 25M2N6 | 8 | 4 | 2 | 5 | 3 | 0 | 6.3618 | 3.2599 | 2.9110 | 0.9975 | 0.288675 | 0.117851 | 0.4398 | 0 | 2 |
| 114 | 34M2C6 | 8 | 4 | 4 | 8 | 3 | 0 | 6.3618 | 3.3474 | 2.3420 | 1.8450 | 0.288675 | 0.117851 | 0.9773 | 0 | 2 |
| 115 | 34M2T6 | 8 | 4 | 4 | 8 | 3 | 0 | 6.3618 | 3.3474 | 2.3420 | 1.8450 | 0.288675 | 0.117851 | 0.9773 | 0 | 2 |
| 116 | 35M2T6 | 8 | 4 | 3 | 6 | 3 | 0 | 6.3618 | 3.2825 | 2.7330 | 1.2230 | 0.288675 | 0.117851 | 0.5261 | 0 | 2 |
| 117 | 35M2T6 | 8 | 4 | 3 | 6 | 3 | 0 | 6.3618 | 3.2825 | 2.7330 | 1.2230 | 0.288675 | 0.117851 | 0.5261 | 0 | 2 |
| 118 | 44M2C6 | 8 | 4 | 3 | 7 | 2 | 0 | 6.3618 | 3.2600 | 2.8421 | 1.5291 | 0.333333 | 0.117851 | 0.6440 | 0 | 4 |
| 119 | 44M2T6 | 8 | 4 | 3 | 7 | 2 | 0 | 6.3618 | 3.2600 | 2.8421 | 1.5291 | 0.333333 | 0.117851 | 0.6440 | 0 | 4 |
| 120 | 45M2C6 | 8 | 4 | 4 | 7 | 2 | 0 | 6.3094 | 3.3094 | 2.6289 | 1.5476 | 0.333333 | 0.111111 | 1.0218 | 0 | 2 |
| 121 | 45M2T6 | 8 | 4 | 4 | 7 | 2 | 0 | 6.3094 | 3.3094 | 2.6289 | 1.5476 | 0.333333 | 0.111111 | 1.0218 | 0 | 2 |

Appendix C (*Continued*)

| Observation no. | Shorthand name | NC | TM | P3S | P3T | NCDB | DBE | XV0 | XV1 | XV2 | XVP3 | XVDB | XVT | XVPC4 | NXP6 | NXC3 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 122 | 55M2C6 | 8 | 4 | 3 | 5 | 2 | 0 | 6.3618 | 3.1725 | 3.3338 | 0.9659 | 0.333333 | 0.117851 | 0.4082 | 0 | 4 |
| 123 | 55M2T6 | 8 | 4 | 3 | 5 | 2 | 0 | 6.3618 | 3.1725 | 3.3338 | 0.9659 | 0.333333 | 0.117851 | 0.4082 | 0 | 4 |
| 124 | 3E3N6 | 8 | 3 | 2 | 7 | 3 | 0 | 6.1987 | 3.5254 | 1.9777 | 1.4010 | 0.288675 | 0.102062 | 0.3907 | 0 | 1 |
| 125 | 22M3C6 | 8 | 4 | 0 | 5 | 2 | 0 | 6.3618 | 3.2374 | 3.1766 | 0.8536 | 0.333333 | 0.117851 | 0.3333 | 0 | 4 |
| 126 | 22M3T6 | 8 | 4 | 0 | 5 | 2 | 0 | 6.3618 | 3.2374 | 3.1766 | 0.8536 | 0.333333 | 0.117851 | 0.3333 | 0 | 4 |
| 127 | 23M3C6 | 8 | 4 | 2 | 7 | 3 | 0 | 6.3618 | 3.3474 | 2.5111 | 1.4368 | 0.288675 | 0.117851 | 0.9065 | 0 | 2 |
| 128 | 23M3T6 | 8 | 4 | 2 | 7 | 3 | 0 | 6.3618 | 3.3474 | 2.5111 | 1.4368 | 0.288675 | 0.117851 | 0.9065 | 0 | 2 |
| 129 | 24M3C6 | 8 | 4 | 1 | 6 | 3 | 0 | 6.3618 | 3.3374 | 2.6106 | 1.1755 | 0.288675 | 0.117851 | 0.4886 | 0 | 2 |
| 130 | 24M3T6 | 8 | 4 | 1 | 6 | 3 | 0 | 6.3618 | 3.3374 | 2.6106 | 1.1755 | 0.288675 | 0.117851 | 0.4886 | 0 | 2 |
| 131 | 25M3C6 | 8 | 4 | 0 | 5 | 2 | 0 | 6.3094 | 3.3094 | 2.8729 | 0.8809 | 0.333333 | 0.111111 | 0.3849 | 0 | 2 |
| 132 | 25M3T6 | 8 | 4 | 0 | 5 | 2 | 0 | 6.3094 | 3.3094 | 2.8729 | 0.8809 | 0.333333 | 0.111111 | 0.3849 | 0 | 2 |
| 133 | 34M3C6 | 8 | 4 | 2 | 8 | 4 | 0 | 6.4142 | 3.3713 | 2.2678 | 1.7892 | 0.250000 | 0.125000 | 0.9571 | 0 | 2 |
| 134 | 34M3T6 | 8 | 4 | 2 | 8 | 4 | 0 | 6.4142 | 3.3713 | 2.2678 | 1.7892 | 0.250000 | 0.125000 | 0.9571 | 0 | 2 |
| 135 | 2NP1N5 | 8 | 2 | 4 | 6 | 2 | 1 | 6.0355 | 3.4749 | 2.2500 | 1.2071 | 0.353553 | 0.088388 | 0.2500 | 1 | 1 |
| 136 | 2IP1N5 | 8 | 3 | 4 | 7 | 2 | 1 | 6.1987 | 3.3576 | 2.5629 | 1.3876 | 0.353553 | 0.102062 | 0.7990 | 0 | 2 |
| 137 | 2E3M1N5 | 8 | 3 | 5 | 8 | 2 | 1 | 6.1987 | 3.3956 | 2.3211 | 1.7634 | 0.353553 | 0.102062 | 0.8835 | 0 | 2 |
| 138 | 2E4M1N5 | 8 | 3 | 4 | 6 | 2 | 1 | 6.1987 | 3.3307 | 2.7015 | 1.1969 | 0.353553 | 0.102062 | 0.4830 | 0 | 2 |
| 139 | 3E2M1N5 | 8 | 3 | 6 | 8 | 2 | 1 | 6.1987 | 3.3729 | 2.3598 | 1.6825 | 0.353553 | 0.102062 | 0.8237 | 0 | 2 |
| 140 | 3E3M1N5 | 8 | 3 | 6 | 9 | 1 | 1 | 6.1987 | 3.3182 | 2.5653 | 2.1082 | 0.408248 | 0.102062 | 0.9433 | 0 | 4 |
| 141 | 3E4M1N5 | 8 | 3 | 6 | 8 | 1 | 1 | 6.1463 | 3.3450 | 2.5518 | 1.6305 | 0.408248 | 0.096225 | 0.9326 | 0 | 2 |
| 142 | 233M1N5 | 8 | 4 | 6 | 9 | 2 | 1 | 6.4142 | 3.1642 | 3.0178 | 2.0392 | 0.353553 | 0.125000 | 1.4357 | 0 | 5 |
| 143 | 234M1N5 | 8 | 4 | 6 | 8 | 2 | 1 | 6.3618 | 3.2076 | 2.8790 | 1.7773 | 0.353553 | 0.117851 | 1.4398 | 0 | 3 |
| 144 | 244M1N5 | 8 | 4 | 4 | 5 | 2 | 1 | 6.4142 | 3.0607 | 3.6945 | 0.8321 | 0.353553 | 0.125000 | 0.4786 | 0 | 5 |
| 145 | 334M1N5 | 8 | 4 | 6 | 9 | 1 | 1 | 6.3618 | 3.1403 | 3.1802 | 2.0141 | 0.408248 | 0.117851 | 1.6464 | 0 | 5 |
| 146 | 344M1N5 | 8 | 4 | 6 | 8 | 1 | 1 | 6.3618 | 3.1076 | 3.3904 | 1.7198 | 0.408248 | 0.117851 | 1.5285 | 0 | 5 |
| 147 | 3E2M2N5 | 8 | 4 | 2 | 8 | 4 | 0 | 6.4142 | 3.3713 | 2.3107 | 1.5607 | 0.250000 | 0.125000 | 0.8536 | 0 | 2 |
| 148 | 3E4M2C5 | 8 | 4 | 3 | 8 | 3 | 0 | 6.3618 | 3.3701 | 2.3718 | 1.5206 | 0.288675 | 0.117851 | 0.8422 | 0 | 2 |
| 149 | 3E4M2T5 | 8 | 4 | 3 | 8 | 3 | 0 | 6.3618 | 3.3701 | 2.3718 | 1.5206 | 0.288675 | 0.117851 | 0.8422 | 0 | 2 |
| 150 | 234M2N5 | 8 | 5 | 2 | 8 | 4 | 0 | 6.5774 | 3.1934 | 2.8377 | 1.6547 | 0.250000 | 0.144338 | 1.4047 | 0 | 3 |
| 151 | 244M2N5 | 8 | 5 | 0 | 5 | 3 | 0 | 6.5774 | 3.0774 | 3.5877 | 0.7217 | 0.288675 | 0.144338 | 0.4330 | 0 | 5 |
| 152 | 344M2C5 | 8 | 5 | 3 | 8 | 3 | 0 | 6.5774 | 3.1160 | 3.2217 | 1.6160 | 0.288675 | 0.144338 | 1.3660 | 0 | 5 |
| 153 | 344M2T5 | 8 | 5 | 3 | 8 | 3 | 0 | 6.5774 | 3.1160 | 3.2217 | 1.6160 | 0.288675 | 0.144338 | 1.3660 | 0 | 5 |
| 154 | 2IP3M1N4 | 8 | 4 | 4 | 8 | 2 | 1 | 6.3618 | 3.2403 | 2.8843 | 1.4832 | 0.353553 | 0.117851 | 1.2130 | 0 | 3 |
| 155 | 2E33N1N4 | 8 | 4 | 4 | 8 | 2 | 1 | 6.4142 | 3.1642 | 3.2071 | 1.4874 | 0.353553 | 0.125000 | 1.2071 | 0 | 5 |
| 156 | 1N9 | 9 | 1 | 5 | 8 | 1 | 1 | 6.5271 | 4.0238 | 2.4916 | 1.5118 | 0.408248 | 0.051031 | 0.0000 | 3 | 0 |
| 157 | 2C9 | 9 | 2 | 4 | 6 | 2 | 0 | 6.6902 | 4.0260 | 2.4184 | 1.4600 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |
| 158 | 2T9 | 9 | 2 | 4 | 6 | 2 | 0 | 6.6902 | 4.0260 | 2.4184 | 1.4600 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |
| 159 | 3C9 | 9 | 2 | 3 | 6 | 2 | 0 | 6.6902 | 4.0640 | 2.3754 | 1.3767 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |
| 160 | 3T9 | 9 | 2 | 3 | 6 | 2 | 0 | 6.6902 | 4.0640 | 2.3754 | 1.3767 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |
| 161 | 4C9 | 9 | 2 | 3 | 6 | 2 | 0 | 6.6902 | 4.0640 | 2.4023 | 1.3464 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |
| 162 | 4T9 | 9 | 2 | 3 | 6 | 2 | 0 | 6.6902 | 4.0640 | 2.4023 | 1.3464 | 0.333333 | 0.058926 | 0.0000 | 3 | 0 |

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