## Title

STRUCTURES OF BICYCLO(2.21) SYSTEMS III. 2-EXO-HYDR0XY-7-METHYLBICYCL0(2.2.1)HEPTANE-7-SYN-CARBOXYLIC ACID.



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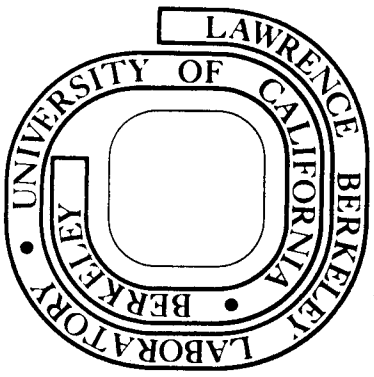

## DISCLAIMER

# Structures of Bicyclo[2.2.1] Systems III.

## 2-exo-hydroxy-7-methylbicyclo[2.2.1]heptane-7-syn-carboxylic acid*

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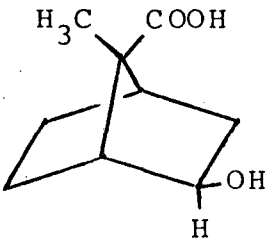
Abstract. $C_9H_{14}O_3$, monoclinic, $P2_1/c$, a = 11.58(2), b = 6.874(10), c = 12.02(2) Å, β = 115.21(5)°, Z = 4, $D_x$ = 1.306(7), $D_m$ = 1.32(1) g $cm^{-3}$, at 22°C. For 798 reflections with I > σ, R = 0.056 and $R_w$ = 0.032. The norbornane skeleton shows no distortion by the substituent groups, and the O(hydroxyl)-C(carboxyl) distance 2.87 Å is less crowded than in a related 2,6-hydroxyacid which lactonizes more rapidly.

* Work done in part with support from the U.S. Energy Research and Development Administration.

Introduction. This compound was studied as part of a program to establish the dimensions and their variation for a variety of substituted norbornane molecules (Chapuis, Zalkin & Templeton, 1973 and 197x). There has been contradiction in the literature concerning the identity of this isomer, and our work directly confirms its assignment by Moriarty & Adams (1973) to the structure:




This hydroxyacid was prepared from the lactone which melts at 125-126° (Storm & Koshland, 1972b) and was crystallized from ethyl acetate by Hackney (1975). Photographic and diffractometer x-ray experiments were made with a crystal 0.16 x 0.14 x 0.03 mm in size. Absent reflections $h0\ell$, $\ell \neq 2n$ and $0k0$, $k \neq 2n$ indicate space group $P2_1/c$. Setting angles of 12 reflections within the range $23° < 2\theta < 28°$ were used for least-squares adjustment of the cell dimensions ($\lambda$ 0.70926 Å for Mo$K\alpha_1$). Intensities were measured by $\theta$-$2\theta$ scan technique for 2293 reflections with $2\theta < 45°$ in the half-sphere with k non-negative. Averaging of equivalent pairs yielded 1146 independent reflections; for 798 of them, $I > \sigma$. With $\mu$(Mo) = 1.0 $cm^{-1}$ an absorption correction was deemed unnecessary. An empirical extinction correction added 13% to the structure factor of the strongest reflection. The structure was solved by the MULTAN program (Germain, Main & Woolfson, 1971). Hydrogen atoms were found in difference maps or by calculation from coordinates of carbon atoms. Atomic form factors, the method of

weighting, and definitions of R and $R_w$ were the same as described before (Chapuis, et al., 197x) except that w = 0 if $I < \sigma$. In the last cycle, no parameter shifted more than 0.15 $\sigma$. The final R was 0.056 for 798 reflections and 0.096 including reflections of zero weight; $R_w$ was 0.032. Final parameters, distances, and angles are listed in Tables 1 - 4.*

Discussion. Figure 1 shows the molecular shape and numbering scheme. The range of C–C bond lengths from 1.51 to 1.56 suggests that the standard deviations are somewhat underestimated by the least-squares method, but otherwise these distances are unremarkable. The bond angles conform closely to the symmetry of unsubstituted norbornane, and they give little indication that the framework has been distorted by the substituent groups. This result is in contrast to the substantial distortion observed in the salt of a 2,6-hydroxyacid (Chapuis, et al., 197x). We note that the distance between O(3) and C(9) is 2.866(8) Å, only modestly greater than the 2.783(3) Å observed for the 2,6-hydroxyacid. Estimates from Dreiding models (Storm & Koshland, 1972a; Moriarty & Adams, 1973) correspond to about 2.9 and 2.2 Å, respectively, for these two distances; these values also indicate that there is considerable strain in the latter compound. The 2,6-compound undergoes acid-catalyzed lactonization with a rate about 7 x $10^4$ times greater than the 2,7-compound (Hackney, 1975). For reference in

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No.

discussions of these rates, we report also the angles C(2) - O(3) - C(9) = 78.7(2)° and C(7) - C(9) - O(3) = 82.0(2)°.

Each molecule is attached to three others by a total of four hydrogen bonds (Fig. 2), forming sheets parallel to (100). Each hydroxyl group forms a hydrogen bond to O(1) of one neighboring molecule while it accepts a hydrogen bond from O(2) of another neighbor.

We thank Dr. D.D. Hackney and Professor D.E. Koshland for providing the crystals. G. Chapuis acknowledges the Swiss National Funds for financial support.

## References

Chapuis, G., Zalkin, A. & Templeton, D.H. (1973). Acta Cryst. B 29, 2642-2644.

Chapuis, G., Zalkin, A. & Templeton, D.H. (197x). Submitted to Acta Crystallographica.

Germain, G., Main, P. & Woolfson, M.M. (1971). Acta Cryst. A 27, 368-376.

Hackney, D.D. (1975). Models for Chymotrypsin and the Interaction of Lysozyme with Urea. Thesis, University of California, Berkeley.

Moriarty, R.M. & Adams, T. (1973). J. Amer. Chem. Soc. 95, 4070-4071.

Storm, D.R. & Koshland, D.E. (1972a). J. Amer. Chem. Soc. 94, 5805-5814.

Storm, D.R. & Koshland, D.E. (1972b). J. Amer. Chem. Soc. 94, 5815-5825.

Table 1. Parameters for heavy atoms[a]

| | x | y | z | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| C(1) | .2123(3) | .1437(6) | .5756(3) | 2.1(2) | 3.1(2) | 1.6(1) | - .1(2) | .7(1) | - .2(2) |
| C(2) | .1376(3) | .2964(6) | .4823(3) | 2.8(2) | 2.3(2) | 2.8(2) | - .1(2) | 1.1(2) | - .3(2) |
| C(3) | .2113(4) | .3148(7) | .4011(4) | 3.7(2) | 3.4(3) | 3.0(2) | - .6(2) | 1.7(2) | .5(2) |
| C(4) | .3218(3) | .1704(5) | .4621(3) | 2.4(2) | 3.8(2) | 2.1(2) | - .1(2) | 1.1(1) | - .6(2) |
| C(5) | .4152(4) | .2563(8) | .5847(4) | 3.3(2) | 4.1(3) | 3.3(2) | - .8(2) | 1.4(2) | - .8(2) |
| C(6) | .3374(4) | .2426(8) | .6633(4) | 3.4(2) | 4.0(3) | 2.7(2) | - .2(2) | .9(2) | - .6(2) |
| C(7) | .2582(3) | .0056(5) | .5018(3) | 1.9(2) | 3.1(2) | 1.7(1) | .1(1) | .5(1) | .2(2) |
| C(8) | .3480(5) | -.1569(7) | .5779(5) | 2.9(2) | 3.9(3) | 3.7(2) | .9(2) | .8(2) | .5(2) |
| C(9) | .1522(3) | -.1019(6) | .3985(3) | 2.5(2) | 2.9(2) | 2.2(2) | .5(2) | 1.0(1) | .2(2) |
| O(1) | .0737(2) | -.2023(4) | .4135(2) | 3.3(1) | 3.8(1) | 3.4(1) | -1.1(1) | 1.8(1) | - .3(1) |
| O(2) | .1595(3) | -.0897(4) | .2917(2) | 3.5(1) | 5.4(2) | 2.5(1) | -1.6(1) | 1.5(1) | -1.1(1) |
| O(3) | .0087(2) | .2341(4) | .4050(2) | 2.5(1) | 4.3(2) | 2.8(1) | .7(1) | 1.0(1) | 1.2(1) |

[a] The form of the temperature factor is $\exp[-0.25(h^2a^{*2}B_{11}+2hka^*b^*B_{12}+\ldots)]$.

Table 2. Parameters for hydrogen atoms[a]

| | x | y | z | B |
|---|---|---|---|---|
| H(1) | .156(3) | .082(4) | .615(3) | 1.7(8) |
| H(2) | .131(3) | .441(5) | .521(3) | 2.6(8) |
| H(3) | .144(3) | .275(5) | .303(3) | 2.5(7) |
| H(4) | .246(3) | .455(6) | .400(3) | 2.6(9) |
| H(5) | .365(3) | .121(4) | .405(2) | 1.4(7) |
| H(6) | .500(3) | .168(5) | .626(3) | 3.3(9) |
| H(7) | .438(4) | .407(7) | .577(4) | 5.4(12) |
| H(8) | .391(3) | .152(5) | .739(3) | 2.4(9) |
| H(9) | .321(3) | .384(6) | .688(3) | 4.0(10) |
| H(10) | .293(4) | -.261(7) | .611(4) | 6.2(12) |
| H(11) | .389(4) | -.236(6) | .525(3) | 5.2(11) |
| H(12) | .428(4) | -.102(6) | .647(3) | 4.0(10) |
| H(13) | .083(5) | -.169(8) | .228(5) | 9.9(18) |
| H(14) | -.038(5) | .217(8) | .459(4) | 9.2(17) |

[a] The form of the temperature factor is $\exp(-B\lambda^{-2}\sin^2\theta)$.

Table 3. Bond distances (Å)

| | | | |
|---|---|---|---|
| C(1)-C(2) | 1.511(6) | C(1)-H(1) | 1.04(3) |
| C(1)-C(6) | 1.540(6) | C(2)-H(2) | 1.11(3) |
| C(1)-C(7) | 1.540(6) | C(3)-H(3) | 1.13(3) |
| C(2)-C(3) | 1.552(6) | C(3)-H(4) | 1.05(4) |
| C(3)-C(4) | 1.537(6) | C(4)-H(5) | 1.06(3) |
| C(4)-C(5) | 1.527(6) | C(5)-H(6) | 1.08(3) |
| C(4)-C(7) | 1.534(6) | C(5)-H(7) | 1.08(4) |
| C(5)-C(6) | 1.561(7) | C(6)-H(8) | 1.06(3) |
| C(7)-C(8) | 1.536(6) | C(6)-H(9) | 1.06(4) |
| C(7)-C(9) | 1.515(6) | C(8)-H(10) | 1.14(5) |
| C(2)-O(3) | 1.447(5) | C(8)-H(11) | 1.09(4) |
| C(9)-O(1) | 1.215(5) | C(8)-H(12) | 1.02(4) |
| C(9)-O(2) | 1.323(5) | O(2)-H(13) | 1.04(5) |
| O(1)...O(3) | 2.737(6) | O(3)-H(14) | 1.01(5) |
| O(2)...O(3) | 2.633(6) | | |

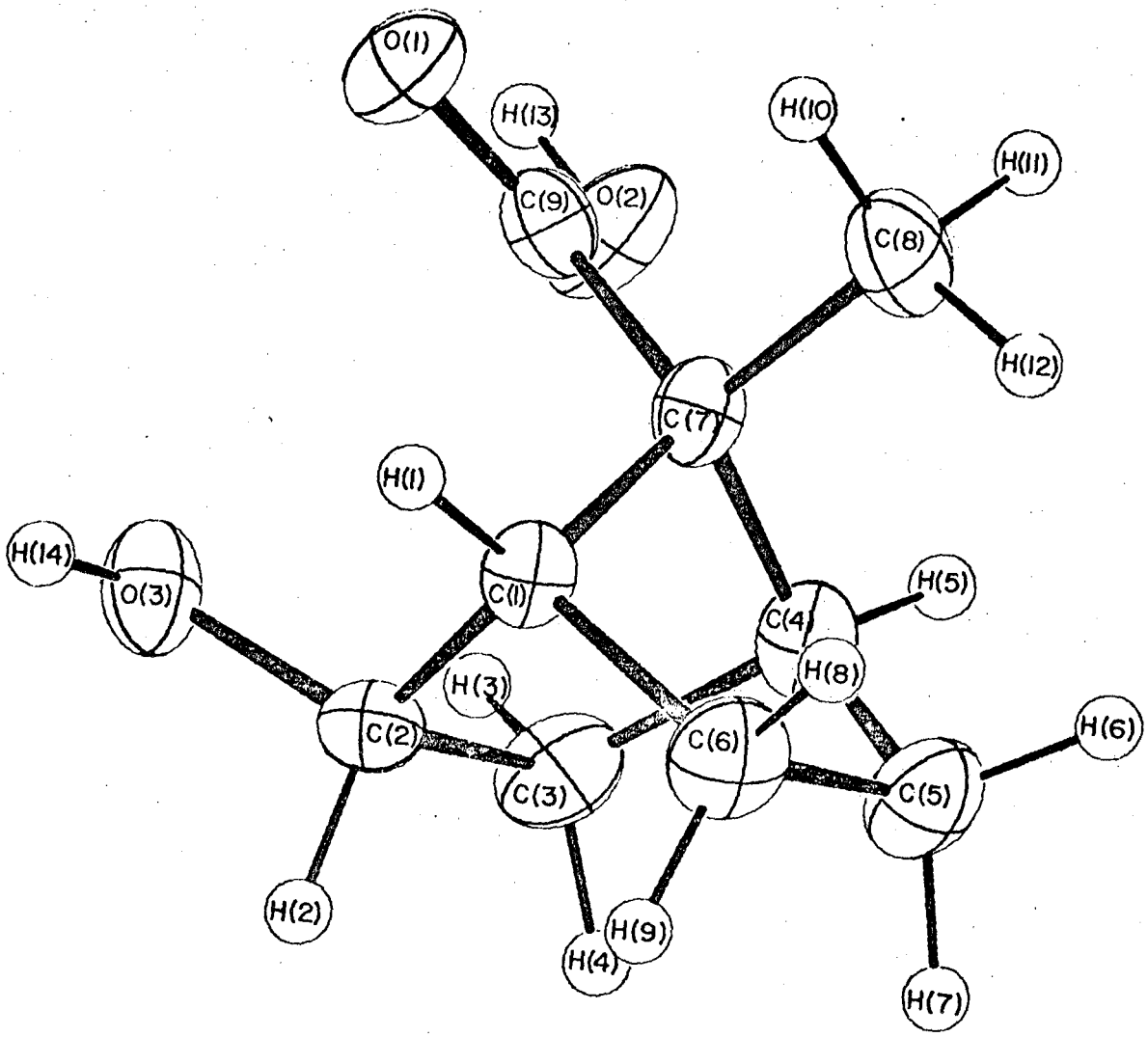
Table 4. Bond angles (deg)

| | |
|---|---|
| C(2)-C(1)-C(6) | 106.0(4) |
| C(2)-C(1)-C(7) | 103.2(3) |
| C(6)-C(1)-C(7) | 102.2(3) |
| C(1)-C(2)-C(3) | 103.3(3) |
| C(1)-C(2)-O(3) | 112.3(3) |
| C(3)-C(2)-O(3) | 108.3(3) |
| C(2)-C(3)-C(4) | 102.5(3) |
| C(3)-C(4)-C(5) | 108.3(4) |
| C(3)-C(4)-C(7) | 102.2(3) |
| C(5)-C(4)-C(7) | 102.8(3) |
| C(4)-C(5)-C(6) | 102.0(3) |
| C(1)-C(6)-C(5) | 103.3(3) |
| C(1)-C(7)-C(4) | 93.1(3) |
| C(1)-C(7)-C(8) | 114.6(3) |
| C(1)-C(7)-C(9) | 114.5(3) |
| C(4)-C(7)-C(8) | 115.4(3) |
| C(4)-C(7)-C(9) | 115.7(3) |
| C(8)-C(7)-C(9) | 103.9(4) |
| C(7)-C(9)-O(1) | 123.4(3) |
| C(7)-C(9)-O(2) | 113.6(3) |
| O(1)-C(9)-O(2) | 122.8(3) |
| C(9)-O(2)-H(13) | 107(2) |
| C(2)-O(3)-H(14) | 108(3) |
| O(1)...O(3)-H(14) | 11(3) |
| O(3)...O(2)-H(13) | 13(3) |

## Figure Captions

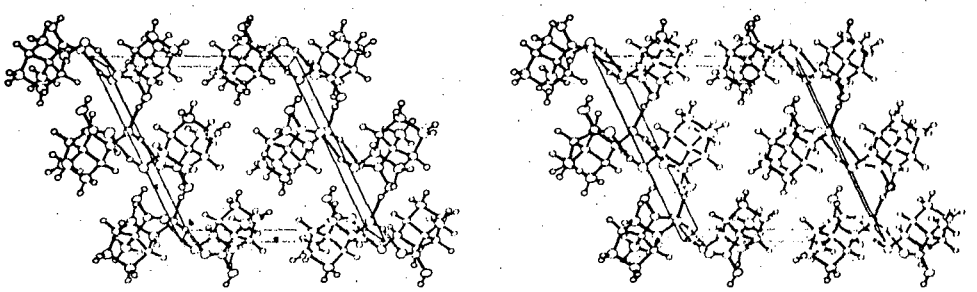
Fig 1. Perspective view of a molecule with 50% probability thermal ellipsoids, drawn with Johnson's ORTEP. Size of hydrogen atoms is arbitrary.

Fig 2. Stereoscopic view of the crystal structure along the b axis, showing hydrogen bonds between molecules.




XBL 741-239

Fig. 1



XBL 741-241

Fig. 2

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X10.0) FOR THE NORBORNANE DERIVATIVE [ C9 H14 O3 ]. F(0,0,0) = 7363

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

| K | FOB | SG | DEL | K | FOB | SG | DEL | K | FOB | SG | DEL | K | FOB | SG | DEL | K | FOB | SG | DEL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H,L= | 0, | 0 | | 1 | 248 | 7 | -6 | 2 | 212 | 22 | 19 | 7 | 7 | 81 | -3* | 2 | 186 | 10 | 1 |
| 2 | 1940 | 20 | 18 | 2 | 250 | 9 | -3 | 3 | 231 | 17 | 1 | H,L= | 1, | 0 | | 3 | 79 | 94 | 5* |
| 4 | 154 | 11 | -15 | 3 | 409 | 6 | -12 | 4 | 148 | 36 | -8 | 0 | 989 | 12 | -14 | 4 | 68 | 93 | -25* |
| 6 | 74 | 98 | 71* | 4 | 59 | 89 | 13* | 5 | 67 | 92 | -10* | 1 | 1010 | 12 | -17 | 5 | 89 | 106 | -35* |
| H,L= | 0, | 1 | | 5 | 88 | 37 | 22 | 6 | 67 | 84 | 49* | 2 | 277 | 21 | -22 | 6 | 46 | 73 | 17* |
| 1 | 1352 | 14 | 15 | H,L= | 0, | 8 | | H,L= | 1, | -6 | | 3 | 609 | 13 | -9 | H,L= | 1, | 7 | |
| 2 | 780 | 11 | -36 | 0 | 177 | 15 | 28 | 0 | 670 | 13 | 5 | 4 | 95 | 19 | 8 | 1 | 127 | 21 | 23 |
| 3 | 462 | 8 | 1 | 1 | 201 | 15 | 3 | 1 | 56 | 21 | 41 | 5 | 70 | 29 | 52 | 2 | 94 | 27 | -8 |
| 4 | 53 | 65 | 9* | 2 | 231 | 20 | 3 | 2 | 262 | 6 | -2 | 6 | 92 | 23 | 5 | 3 | 64 | 77 | 36* |
| 5 | 48 | 58 | 13* | 3 | 260 | 13 | 20 | 3 | 69 | 82 | 4* | 7 | 128 | 29 | 16 | 4 | 54 | 56 | 50* |
| 6 | 50 | 53 | 30* | 4 | 148 | 35 | 5 | 4 | 129 | 44 | 28 | H,L= | 1, | 1 | | 5 | 0 | 90 | -14* |
| 7 | 155 | 22 | 3 | 5 | 92 | 100 | 13* | 5 | 89 | 95 | -2* | 1 | 331 | 8 | -11 | H,L= | 1, | 8 | |
| H,L= | 0, | 2 | | H,L= | 0, | 9 | | 6 | 51 | 117 | -30* | 2 | 187 | 21 | -2 | 0 | 75 | 43 | -11 |
| 0 | 1980 | 21 | 45 | 1 | 203 | 21 | 2 | H,L= | 1, | -5 | | 3 | 137 | 16 | 27 | 1 | 50 | 68 | 18* |
| 1 | 288 | 17 | -21 | 2 | 264 | 9 | -5 | 1 | 116 | 43 | -11 | 4 | 150 | 25 | -2 | 2 | 136 | 12 | 1 |
| 2 | 674 | 11 | -15 | 3 | 178 | 10 | -7 | 2 | 246 | 16 | 11 | 5 | 200 | 20 | -11 | 3 | 148 | 29 | -10 |
| 3 | 293 | 12 | -10 | 4 | 80 | 95 | 54* | 3 | 207 | 24 | 7 | 6 | 138 | 46 | -13 | 4 | 28 | 57 | 5* |
| 4 | 228 | 10 | -7 | H,L= | 0, | 10 | | 4 | 35 | 86 | 11* | 7 | 138 | 27 | 18 | 5 | 107 | 79 | 14 |
| 5 | 55 | 85 | -51* | 0 | 526 | 14 | -9 | 5 | 202 | 19 | -18 | H,L= | 1, | 2 | | H,L= | 1, | 9 | |
| 6 | 239 | 12 | -3 | 1 | 243 | 26 | -4 | 6 | 80 | 49 | 57 | 0 | 382 | 11 | -16 | 1 | 118 | 25 | 22 |
| 7 | 173 | 17 | -1 | 2 | 87 | 102 | 72* | H,L= | 1, | -4 | | 1 | 299 | 19 | -20 | 2 | 366 | 10 | 10 |
| H,L= | 0, | 3 | | 3 | 181 | 14 | 12 | 0 | 225 | 20 | 10 | 2 | 246 | 15 | 31 | 3 | 150 | 25 | -12 |
| 1 | 68 | 112 | 20* | H,L= | 0, | 11 | | 1 | 56 | 86 | 1* | 3 | 865 | 10 | 6 | 4 | 79 | 46 | 28 |
| 2 | 102 | 42 | -40 | 1 | 116 | 129 | -2* | 2 | 501 | 8 | -2 | 4 | 58 | 59 | -5* | H,L= | 1, | 10 | |
| 3 | 242 | 8 | 3 | 2 | 130 | 48 | 41 | 3 | 82 | 44 | 31 | 5 | 323 | 14 | 5 | 0 | 598 | 8 | -7 |
| 4 | 179 | 22 | 20 | H,L= | 1, | -12 | | 4 | 225 | 15 | 5 | 6 | 0 | 96 | -11* | 1 | 96 | 41 | 14 |
| 5 | 140 | 31 | -2 | 0 | 227 | 16 | 13 | 5 | 121 | 32 | 0 | 7 | 131 | 60 | -10 | 2 | 228 | 21 | -23 |
| 6 | 0 | 63 | -26* | 1 | 173 | 22 | 19 | 6 | 0 | 63 | -32* | H,L= | 1, | 3 | | 3 | 131 | 33 | 22 |
| 7 | 188 | 22 | -1 | H,L= | 1, | -11 | | 7 | 73 | 86 | 38* | 1 | 658 | 10 | -1 | H,L= | 1, | 11 | |
| H,L= | 0, | 4 | | 1 | 92 | 22 | -20 | H,L= | 1, | -3 | | 2 | 851 | 9 | 10 | 1 | 136 | 47 | -23 |
| 0 | 676 | 9 | 5 | 2 | 168 | 17 | 6 | 1 | 83 | 98 | -9* | 3 | 328 | 13 | -20 | H,L= | 2, | -12 | |
| 1 | 554 | 8 | 10 | 3 | 82 | 103 | 72* | 2 | 138 | 39 | -1 | 4 | 142 | 23 | -17 | 0 | 186 | 17 | 31 |
| 2 | 797 | 15 | 21 | H,L= | 1, | -10 | | 3 | 86 | 28 | 23 | 5 | 15 | 80 | -22* | 1 | 30 | 91 | 9* |
| 3 | 89 | 72 | 27 | 0 | 0 | 64 | -15* | 4 | 378 | 10 | -13 | 6 | 77 | 91 | 4* | 2 | 103 | 37 | 31 |
| 4 | 67 | 76 | 54* | 1 | 91 | 114 | -4* | 5 | 41 | 85 | 11* | 7 | 85 | 53 | 60 | H,L= | 2, | -11 | |
| 5 | 58 | 67 | 43* | 2 | 53 | 69 | 30* | 6 | 90 | 59 | -9 | H,L= | 1, | 4 | | 1 | 116 | 73 | -24 |
| 6 | 138 | 30 | -25 | 3 | 122 | 20 | 29 | 7 | 138 | 22 | 17 | 0 | 135 | 19 | 5 | 2 | 15 | 78 | 6* |
| H,L= | 0, | 5 | | 4 | 68 | 82 | -14* | H,L= | 1, | -2 | | 1 | 71 | 17 | 4 | 3 | 224 | 10 | 2 |
| 1 | 47 | 48 | 8* | H,L= | 1, | -9 | | 0 | 0 | 124 | -0* | 2 | 158 | 16 | 10 | H,L= | 2, | -10 | |
| 2 | 0 | 70 | -46* | 1 | 127 | 17 | 25 | 1 | 858 | 10 | -21 | 3 | 131 | 15 | 7 | 0 | 106 | 68 | 25 |
| 3 | 513 | 13 | -5 | 2 | 73 | 78 | -21* | 2 | 575 | 9 | -12 | 4 | 193 | 12 | 6 | 1 | 62 | 91 | -22* |
| 4 | 52 | 62 | 10* | 3 | 114 | 25 | 35 | 3 | 425 | 5 | -1 | 5 | 280 | 17 | 19 | 2 | 446 | 7 | 5 |
| 5 | 56 | 74 | 30* | 4 | 93 | 60 | 40 | 4 | 285 | 11 | -2 | 6 | 41 | 82 | 22* | 3 | 124 | 76 | -39 |
| 6 | 53 | 109 | 30* | 5 | 31 | 81 | -33* | 5 | 228 | 11 | -0 | H,L= | 1, | 5 | | 4 | 110 | 37 | -30 |
| H,L= | 0, | 6 | | H,L= | 1, | -8 | | 6 | 70 | 72 | 52* | 1 | 103 | 15 | 14 | H,L= | 2, | -9 | |
| 0 | 847 | 14 | -2 | 0 | 254 | 10 | -15 | 7 | 29 | 77 | 25* | 2 | 315 | 7 | 3 | 1 | 126 | 32 | 9 |
| 1 | 35 | 48 | 3* | 1 | 49 | 67 | 11* | H,L= | 1, | -1 | | 3 | 279 | 15 | -6 | 2 | 412 | 13 | -3 |
| 2 | 554 | 7 | 7 | 2 | 15 | 82 | 12* | 1 | 178 | 30 | -29 | 4 | 318 | 14 | -9 | 3 | 468 | 9 | 0 |
| 3 | 151 | 21 | -3 | 3 | 200 | 18 | -6 | 2 | 1077 | 12 | -8 | 5 | 152 | 35 | -14 | 4 | 102 | 30 | 98 |
| 4 | 197 | 15 | 14 | 4 | 11 | 95 | -61* | 3 | 157 | 17 | 17 | 6 | 132 | 14 | 6 | 5 | 165 | 27 | 26 |
| 5 | 91 | 75 | 11 | 5 | 0 | 74 | -29* | 4 | 93 | 20 | -23 | H,L= | 1, | 6 | | H,L= | 2, | -8 | |
| 6 | 0 | 65 | -37* | H,L= | 1, | -7 | | 5 | 151 | 39 | -9 | 0 | 185 | 10 | -7 | 0 | 518 | 8 | -2 |
| H,L= | 0, | 7 | | 1 | 277 | 6 | -2 | 6 | 75 | 89 | -36* | 1 | 302 | 14 | -10 | 1 | 132 | 11 | -5 |

STRUCTURE FACTORS CONTINUED FOR
THE NORBORNANE DERIVATIVE [ C9 H14 O3 ].

| K | FOB | SG | DEL |
|---|---|---|---|
| 2 | 159 | 46 | 8 |
| 3 | 214 | 11 | -2 |
| 4 | 319 | 18 | -15 |
| 5 | 76 | 89 | -39* |
| H,L= | 2, | -7 | |
| 1 | 175 | 19 | -1 |
| 2 | 92 | 22 | -1 |
| 3 | 402 | 7 | -9 |
| 4 | 242 | 7 | 11 |
| 5 | 121 | 42 | 13 |
| 6 | 79 | 94 | 64* |
| H,L= | 2, | -6 | |
| 0 | 523 | 7 | 1 |
| 1 | 179 | 11 | -0 |
| 2 | 140 | 10 | 11 |
| 3 | 33 | 77 | -6* |
| 4 | 467 | 10 | -14 |
| 5 | 133 | 37 | 9 |
| 6 | 128 | 23 | -14 |
| H,L= | 2, | -5 | |
| 1 | 391 | 8 | 3 |
| 2 | 253 | 10 | -3 |
| 3 | 106 | 33 | 30 |
| 4 | 92 | 26 | 15 |
| 5 | 201 | 32 | -22 |
| 6 | 74 | 46 | 5 |
| H,L= | 2, | -4 | |
| 0 | 698 | 9 | -8 |
| 1 | 45 | 72 | 3* |
| 2 | 421 | 7 | -2 |
| 3 | 300 | 8 | 6 |
| 4 | 445 | 9 | 7 |
| 5 | 161 | 23 | -17 |
| 6 | 63 | 118 | 3* |
| 7 | 183 | 14 | 34 |
| H,L= | 2, | -3 | |
| 1 | 210 | 32 | -29 |
| 2 | 260 | 13 | -26 |
| 3 | 0 | 50 | -0* |
| 4 | 149 | 19 | -16 |
| 5 | 171 | 35 | -48 |
| 6 | 125 | 22 | 23 |
| 7 | 63 | 73 | -4* |
| H,L= | 2, | -2 | |
| 0 | 2567 | 26 | 170 |
| 1 | 472 | 13 | -19 |
| 2 | 354 | 11 | -11 |
| 3 | 285 | 5 | 5 |
| 4 | 52 | 62 | 2* |
| 5 | 102 | 25 | -25 |
| 6 | 111 | 32 | 13 |
| 7 | 168 | 33 | 18 |
| H,L= | 2, | -1 | |
| 1 | 1127 | 11 | -15 |
| 2 | 172 | 35 | -25 |
| 3 | 107 | 12 | 3 |
| 4 | 265 | 6 | -1 |
| 5 | 242 | 18 | -7 |
| 6 | 186 | 21 | 3 |
| 7 | 137 | 28 | -3 |
| H,L= | 2, | 0 | |
| 0 | 978 | 10 | -25 |
| 1 | 761 | 9 | -3 |
| 2 | 659 | 9 | -6 |
| 3 | 97 | 14 | 4 |
| 4 | 357 | 15 | -4 |
| 5 | 204 | 25 | -17 |
| 6 | 245 | 21 | 16 |
| 7 | 149 | 31 | -20 |
| H,L= | 2, | 1 | |
| 1 | 58 | 91 | 27* |
| 2 | 818 | 11 | -5 |
| 3 | 347 | 11 | 4 |
| 4 | 154 | 20 | -14 |
| 5 | 49 | 67 | 38* |
| 6 | 133 | 61 | -31 |
| 7 | 253 | 24 | 17 |
| H,L= | 2, | 2 | |
| 0 | 1414 | 16 | 13 |
| 1 | 339 | 15 | -9 |
| 2 | 1017 | 12 | 10 |
| 3 | 69 | 82 | -5* |
| 4 | 188 | 11 | -1 |
| 5 | 68 | 91 | -21* |
| 6 | 376 | 11 | 10 |
| 7 | 103 | 103 | -54* |
| H,L= | 2, | 3 | |
| 1 | 410 | 7 | 19 |
| 2 | 111 | 22 | 19 |
| 3 | 80 | 41 | 42 |
| 4 | 218 | 17 | 27 |
| 5 | 207 | 10 | 14 |
| 6 | 45 | 58 | -13* |
| H,L= | 2, | 4 | |
| 0 | 341 | 8 | 7 |
| 1 | 488 | 7 | 3 |
| 2 | 259 | 10 | 4 |
| 3 | 266 | 25 | -16 |
| 4 | 133 | 23 | 3 |
| 5 | 127 | 45 | 13 |
| 6 | 40 | 78 | 34* |
| H,L= | 2, | 5 | |
| 1 | 249 | 16 | -11 |
| 2 | 175 | 12 | -4 |
| 3 | 95 | 25 | -25 |
| 4 | 72 | 54 | 1 |
| 5 | 309 | 14 | 8 |
| 6 | 0 | 61 | -33* |
| H,L= | 2, | 6 | |
| 0 | 286 | 8 | -2 |
| 1 | 149 | 19 | 12 |
| 2 | 268 | 11 | 16 |
| 3 | 160 | 9 | 13 |
| 4 | 353 | 15 | -11 |
| 5 | 130 | 33 | -4 |
| H,L= | 2, | 7 | |
| 1 | 115 | 20 | -3 |
| 2 | 154 | 55 | -10 |
| 3 | 0 | 67 | -17* |
| 4 | 27 | 74 | -28* |
| 5 | 171 | 12 | -10 |
| H,L= | 2, | 8 | |
| 0 | 372 | 8 | -6 |
| 1 | 155 | 23 | -24 |
| 2 | 96 | 23 | 1 |
| 3 | 102 | 45 | 79 |
| 4 | 58 | 80 | -1* |
| H,L= | 2, | 9 | |
| 1 | 195 | 15 | -8 |
| 2 | 31 | 57 | -3* |
| 3 | 67 | 75 | -3* |
| H,L= | 2, | 10 | |
| 0 | 103 | 53 | -15 |
| 1 | 63 | 75 | -4* |
| 2 | 92 | 109 | 1* |
| H,L= | 3, | -12 | |
| 0 | 126 | 26 | 3 |
| 1 | 63 | 69 | 37* |
| 2 | 0 | 107 | -24* |
| H,L= | 3, | -11 | |
| 1 | 54 | 76 | 44* |
| 2 | 98 | 20 | -18 |
| 3 | 70 | 83 | 1* |
| H,L= | 3, | -10 | |
| 0 | 244 | 21 | 4 |
| 1 | 113 | 26 | 27 |
| 2 | 0 | 89 | -35* |
| 3 | 58 | 78 | 51* |
| 4 | 87 | 104 | 23* |
| H,L= | 3, | -9 | |
| 1 | 89 | 94 | 58* |
| 2 | 180 | 14 | 8 |
| 3 | 262 | 8 | -6 |
| 4 | 174 | 53 | 4 |
| 5 | 258 | 23 | 6 |
| H,L= | 3, | -8 | |
| 0 | 77 | 79 | 48* |
| 1 | 345 | 17 | 8 |
| 2 | 160 | 14 | -12 |
| 3 | 0 | 72 | -24* |
| 4 | 130 | 21 | -2 |
| 5 | 235 | 16 | -7 |
| H,L= | 3, | -7 | |
| 1 | 410 | 9 | -1 |
| 2 | 113 | 17 | 11 |
| 3 | 218 | 12 | 2 |
| 4 | 124 | 47 | -38 |
| 5 | 76 | 25 | 47 |
| 6 | 0 | 66 | -2* |
| H,L= | 3, | -6 | |
| 0 | 90 | 91 | -30* |
| 1 | 524 | 6 | 3 |
| 2 | 247 | 6 | -4 |
| 3 | 219 | 16 | 16 |
| 4 | 180 | 21 | 26 |
| 5 | 241 | 9 | -4 |
| 6 | 80 | 96 | 51* |
| H,L= | 3, | -5 | |
| 1 | 228 | 6 | -9 |
| 2 | 524 | 8 | -2 |
| 3 | 139 | 28 | -5 |
| 4 | 286 | 9 | 20 |
| 5 | 56 | 69 | 35* |
| 6 | 109 | 41 | 59 |
| H,L= | 3, | -4 | |
| 0 | 478 | 10 | -11 |
| 1 | 1110 | 14 | -13 |
| 2 | 487 | 8 | 4 |
| 3 | 264 | 20 | -8 |
| 4 | 213 | 9 | -7 |
| 5 | 161 | 15 | 3 |
| 6 | 52 | 73 | -13* |
| 7 | 87 | 104 | 83* |
| H,L= | 3, | -3 | |
| 1 | 185 | 22 | -20 |
| 2 | 546 | 6 | -16 |
| 3 | 225 | 7 | 6 |
| 4 | 275 | 13 | 4 |
| 5 | 200 | 21 | 7 |
| 6 | 62 | 73 | -15* |
| 7 | 0 | 61 | -11* |
| H,L= | 3, | -2 | |
| 0 | 361 | 14 | -20 |
| 1 | 531 | 15 | -14 |
| 2 | 111 | 47 | 0 |
| 3 | 328 | 9 | 6 |
| 4 | 39 | 57 | 25* |
| 5 | 94 | 53 | 42 |
| 6 | 75 | 34 | 63 |
| 7 | 118 | 27 | -19 |
| H,L= | 3, | -1 | |
| 1 | 90 | 102 | -7* |
| 2 | 338 | 7 | 5 |
| 3 | 287 | 14 | -12 |
| 4 | 219 | 15 | -5 |
| 5 | 353 | 11 | -2 |
| 6 | 120 | 24 | 20 |
| 7 | 53 | 63 | 34* |
| H,L= | 3, | 0 | |
| 0 | 69 | 137 | -19* |
| 1 | 476 | 9 | -7 |
| 2 | 811 | 11 | -5 |
| 3 | 242 | 10 | -1 |
| 4 | 458 | 7 | 9 |
| 5 | 207 | 25 | 2 |
| 6 | 84 | 96 | 12* |
| H,L= | 3, | 1 | |
| 1 | 143 | 28 | 26 |
| 2 | 401 | 13 | 11 |
| 2 | 1296 | 15 | 18 |
| 3 | 599 | 8 | 0 |
| 4 | 197 | 7 | 4 |
| 5 | 452 | 9 | -16 |
| 6 | 84 | 95 | 58* |
| 7 | 66 | 48 | -19 |
| H,L= | 3, | 2 | |
| 0 | 467 | 6 | -1 |
| 1 | 722 | 10 | 5 |
| 2 | 50 | 85 | -1* |
| 3 | 346 | 5 | 3 |
| 4 | 112 | 57 | -29 |
| 5 | 163 | 17 | -31 |
| 6 | 52 | 86 | 9* |
| H,L= | 3, | 3 | |
| 1 | 673 | 13 | 16 |
| 2 | 638 | 9 | 1 |
| 3 | 456 | 8 | -8 |
| 4 | 441 | 11 | 9 |
| 5 | 101 | 17 | 18 |
| 6 | 85 | 86 | 24* |
| H,L= | 3, | 4 | |
| 0 | 136 | 10 | 7 |
| 1 | 299 | 9 | -6 |
| 2 | 200 | 19 | -3 |
| 3 | 219 | 11 | -0 |
| 4 | 261 | 11 | -19 |
| 5 | 60 | 74 | -14* |
| 6 | 122 | 51 | -14 |
| H,L= | 3, | 5 | |
| 1 | 6 | 49 | -23* |
| 2 | 149 | 25 | -15 |
| 3 | 0 | 68 | -6* |
| 4 | 73 | 88 | -1* |
| 5 | 50 | 82 | 40* |
| H,L= | 3, | 6 | |
| 0 | 67 | 53 | 21 |
| 1 | 139 | 22 | 0 |
| 2 | 175 | 11 | 4 |
| 3 | 85 | 45 | -5 |
| 4 | 83 | 33 | 16 |
| 5 | 119 | 33 | 51 |
| H,L= | 3, | 7 | |
| 1 | 74 | 51 | 16 |
| 2 | 185 | 21 | 11 |
| 3 | 213 | 23 | 36 |
| 4 | 191 | 105 | 5* |
| H,L= | 3, | 8 | |
| 0 | 159 | 13 | 25 |
| 1 | 376 | 13 | 16 |
| 2 | 101 | 55 | 4 |
| 3 | 0 | 81 | -18* |
| 4 | 0 | 61 | -18* |
| H,L= | 3, | 9 | |
| 1 | 205 | 17 | 33 |
| 2 | 141 | 39 | -17 |

STRUCTURE FACTORS CONTINUED FOR
THE NORBORNANE DERIVATIVE [ C9 H14 O3 ].

| K | FOB | SG | DEL |
|---|---|---|---|
| 3 | 166 | 57 | 21 |
| H,L= | 3, | 10 | |
| 0 | 188 | 29 | -17 |
| H,L= | 4, | -12 | |
| 0 | 215 | 16 | 8 |
| 1 | 149 | 20 | -1 |
| 2 | 129 | 25 | 2 |
| H,L= | 4, | -11 | |
| 1 | 148 | 20 | -5 |
| 2 | 111 | 16 | -0 |
| 3 | 132 | 27 | 11 |
| H,L= | 4, | -10 | |
| 0 | 254 | 16 | 19 |
| 1 | 325 | 18 | 13 |
| 2 | 50 | 99 | -58* |
| 3 | 458 | 8 | -2 |
| 4 | 198 | 39 | -26 |
| H,L= | 4, | -9 | |
| 1 | 101 | 43 | 8 |
| 2 | 179 | 12 | -16 |
| 3 | 62 | 93 | 17* |
| 4 | 59 | 70 | -26* |
| 5 | 256 | 28 | -19 |
| H,L= | 4, | -8 | |
| 0 | 212 | 11 | -10 |
| 1 | 388 | 13 | -8 |
| 2 | 209 | 16 | -10 |
| 3 | 105 | 75 | 14 |
| 4 | 395 | 16 | 1 |
| 5 | 178 | 19 | 2 |
| H,L= | 4, | -7 | |
| 1 | 381 | 17 | -6 |
| 2 | 77 | 86 | 18* |
| 3 | 33 | 82 | -8* |
| 4 | 279 | 17 | -9 |
| 5 | 184 | 13 | -4 |
| 6 | 79 | 58 | 25 |
| H,L= | 4, | -6 | |
| 0 | 107 | 41 | -10 |
| 1 | 445 | 13 | -5 |
| 2 | 626 | 9 | 9 |
| 3 | 16 | 91 | -9* |
| 4 | 97 | 37 | 26 |
| 5 | 371 | 10 | -12* |
| 6 | 23 | 59 | -2* |
| H,L= | 4, | -5 | |
| 1 | 218 | 10 | -4 |
| 2 | 268 | 7 | 3 |
| 3 | 250 | 17 | 14 |
| 4 | 58 | 68 | -38* |
| 5 | 0 | 70 | -33* |
| 6 | 9 | 111 | 4* |
| H,L= | 4, | | -4 |
| | 4 | | 25 |
| 1 | 440 | 8 | 3 |
| 2 | 939 | 10 | 9 |
| 3 | 324 | 7 | -4 |
| 4 | 90 | 48 | 3 |
| 5 | 83 | 29 | 6 |
| 6 | 106 | 65 | 16 |
| H,L= | 4, | -3 | |
| 1 | 191 | 8 | -3 |
| 2 | 443 | 9 | 3 |
| 3 | 510 | 9 | 4 |
| 4 | 118 | 32 | 21 |
| 5 | 120 | 50 | 18 |
| 6 | 104 | 28 | -3 |
| H,L= | 4, | -2 | |
| 0 | 225 | 14 | 4 |
| 1 | 561 | 03 | -40* |
| 2 | 627 | 10 | -0 |
| 3 | 259 | 16 | -2 |
| 4 | 59 | 69 | 51* |
| 5 | 275 | 17 | 10 |
| 6 | 0 | 67 | -39* |
| 7 | 113 | 25 | 20 |
| H,L= | 4, | -1 | |
| 1 | 113 | 55 | -24 |
| 2 | 272 | 9 | 1 |
| 3 | 390 | 11 | 9 |
| 4 | 186 | 16 | 5 |
| 5 | 55 | 65 | 15* |
| 6 | 64 | 82 | -3* |
| 7 | 77 | 100 | 62* |
| H,L= | 4, | 0 | |
| 0 | 563 | 7 | -8 |
| 1 | 437 | 6 | -4 |
| 2 | 233 | 15 | 24 |
| 3 | 392 | 5 | 1 |
| 4 | 264 | 17 | 9 |
| 5 | 132 | 14 | 20 |
| 6 | 129 | 25 | -19 |
| H,L= | 4, | 1 | |
| 1 | 29 | 65 | -4* |
| 2 | 52 | 73 | -1* |
| 3 | 0 | 75 | -14* |
| 4 | 30 | 54 | -4* |
| 5 | 405 | 12 | -5 |
| 6 | 81 | 44 | 60 |
| H,L= | 4, | 2 | |
| 0 | 305 | 16 | -2 |
| 1 | 949 | 10 | 7 |
| 2 | 98 | 19 | 12 |
| 3 | 248 | 8 | -0 |
| 4 | 178 | 11 | -25 |
| 5 | 307 | 10 | 4 |
| 6 | 60 | 44 | 17 |
| H,L= | 4, | 3 | |
| 1 | 618 | 8 | -1 |
| 2 | 154 | 22 | -1 |
| 3 | 257 | 14 | 4 |
| 4 | 122 | 14 | -5 |
| 5 | 248 | 19 | 19 |
| 6 | 81 | 96 | 67* |
| H,L= | 4, | -4 | |
| 0 | 490 | 12 | -6 |
| 1 | 241 | 7 | -10 |
| 2 | 24 | 58 | 10* |
| 3 | 186 | 22 | -11 |
| 4 | 121 | 20 | 64 |
| 5 | 205 | 16 | -19 |
| 6 | 91 | 107 | 60* |
| H,L= | 4, | 5 | |
| 1 | 218 | 33 | -14 |
| 2 | 276 | 23 | -23 |
| 3 | 196 | 24 | 54 |
| 4 | 152 | 61 | 8 |
| 5 | 169 | 37 | 1 |
| H,L= | 4, | 6 | |
| 0 | 51 | 70 | 30* |
| 1 | 590 | 9 | -4 |
| 2 | 235 | 10 | 7 |
| 3 | 264 | 10 | -1 |
| 4 | 61 | 103 | -4* |
| 5 | 34 | 88 | -39* |
| H,L= | 4, | 7 | |
| 1 | 224 | 8 | -6 |
| 2 | 45 | 92 | -21* |
| 3 | 51 | 85 | 10* |
| 4 | 39 | 99 | -34* |
| H,L= | 4, | 8 | |
| 0 | 122 | 24 | 12 |
| 1 | 257 | 15 | 2 |
| 2 | 224 | 25 | 5 |
| 3 | 52 | 76 | 8* |
| H,L= | 4, | 9 | |
| 1 | 76 | 41 | 23 |
| H,L= | 5, | -12 | |
| 0 | 236 | 16 | -2 |
| 1 | 93 | 120 | -6* |
| 2 | 138 | 16 | 11 |
| H,L= | 5, | -11 | |
| 1 | 130 | 25 | -30 |
| 2 | 102 | 121 | 27* |
| 3 | 70 | 48 | 6 |
| H,L= | 5, | -10 | |
| 0 | 615 | 8 | 2 |
| 1 | 138 | 30 | -2 |
| 2 | 326 | 7 | -6 |
| 3 | 195 | 19 | 4 |
| 4 | 77 | 92 | 28* |
| H,L= | 5, | -9 | |
| 1 | 84 | 99 | 1* |
| 2 | 233 | 8 | -10 |
| 3 | 65 | 77 | -6* |
| 4 | 105 | 118 | 2* |
| 5 | 94 | 51 | -15 |
| H,L= | 5, | -8 | |
| 0 | 133 | 25 | 35 |
| 1 | 342 | 10 | 10 |
| 2 | 284 | 8 | -1 |
| 3 | 128 | 62 | -4 |
| 4 | 120 | 62 | 12 |
| 5 | 0 | 71 | -69* |
| H,L= | 5, | -7 | |
| 1 | 121 | 31 | 13 |
| 2 | 244 | 16 | -6 |
| 3 | 51 | 75 | -15* |
| 4 | 145 | 43 | 35 |
| 5 | 144 | 33 | -14 |
| 6 | 117 | 18 | -11 |
| H,L= | 5, | -6 | |
| 0 | 216 | 11 | 3 |
| 1 | 967 | 10 | 4 |
| 2 | 177 | 23 | -25 |
| 3 | 122 | 17 | 7 |
| 4 | 92 | 93 | 27* |
| 5 | 82 | 90 | 33* |
| 6 | 82 | 47 | 48 |
| H,L= | 5, | -5 | |
| 1 | 110 | 19 | 23 |
| 2 | 41 | 74 | 17* |
| 3 | 103 | 27 | 22 |
| 4 | 25 | 86 | 15* |
| 5 | 38 | 75 | 14* |
| 6 | 230 | 16 | -21 |
| H,L= | 5, | -4 | |
| 0 | 720 | 8 | 7 |
| 1 | 225 | 13 | 6 |
| 2 | 110 | 27 | -6 |
| 3 | 67 | 79 | 1* |
| 4 | 0 | 84 | -7* |
| 5 | 172 | 14 | -3 |
| 6 | 48 | 60 | -19* |
| H,L= | 5, | -3 | |
| 1 | 232 | 5 | 1 |
| 2 | 235 | 17 | 7 |
| 3 | 129 | 15 | 18 |
| 4 | 154 | 13 | 7 |
| 5 | 100 | 23 | 16 |
| 6 | 228 | 9 | 6 |
| H,L= | 5, | -2 | |
| 0 | 89 | 100 | 3* |
| 1 | 206 | 10 | -6 |
| 2 | 261 | 12 | 7 |
| 3 | 414 | 8 | -0 |
| 4 | 186 | 15 | 11 |
| 5 | 153 | 20 | 28 |
| 6 | 179 | 15 | 27 |
| H,L= | 5, | -1 | |
| 1 | 299 | 8 | 9 |
| 2 | 67 | 72 | 6* |
| 3 | 133 | 12 | 6 |
| 4 | 75 | 77 | 14* |
| 5 | 354 | 9 | -9 |
| 6 | 80 | 82 | 50* |
| H,L= | 5, | 0 | |
| 0 | 430 | 14 | 16 |
| 1 | 0 | 52 | -29* |
| 2 | 200 | 7 | -3 |
| 3 | 510 | 7 | -3 |
| 4 | 121 | 11 | -37* |
| 5 | 84 | 100 | 63* |
| 6 | 122 | 31 | 29 |
| H,L= | 5, | 1 | |
| 1 | 295 | 9 | -0 |
| 2 | 336 | 8 | 2 |
| 3 | 0 | 86 | -4* |
| 4 | 99 | 29 | -1 |
| 5 | 51 | 61 | 19* |
| 6 | 148 | 70 | 19 |
| H,L= | 5, | 2 | |
| 0 | 38 | 72 | 7* |
| 1 | 338 | 14 | -8 |
| 2 | 393 | 11 | 8 |
| 3 | 179 | 18 | -3 |
| 4 | 234 | 10 | 3 |
| 5 | 82 | 89 | -21* |
| 6 | 78 | 89 | 77* |
| H,L= | 5, | 3 | |
| 1 | 0 | 66 | -39* |
| 2 | 59 | 63 | 51* |
| 3 | 63 | 89 | 7* |
| 4 | 62 | 94 | -57* |
| 5 | 122 | 26 | 27 |
| H,L= | 5, | 4 | |
| 0 | 269 | 7 | 1 |
| 1 | 152 | 20 | -10 |
| 2 | 211 | 14 | 7 |
| 3 | 105 | 24 | 27 |
| 4 | 140 | 17 | 28 |
| 5 | 0 | 68 | -3* |
| H,L= | 5, | 5 | |
| 1 | 72 | 86 | 33* |
| 2 | 90 | 32 | -67 |
| 3 | 125 | 42 | 9 |
| 4 | 52 | 75 | -8* |
| 5 | 61 | 73 | -21* |
| H,L= | 5, | 6 | |
| 0 | 583 | 8 | -11 |
| 1 | 108 | 23 | 43 |
| 2 | 223 | 13 | -8 |
| 3 | 36 | 66 | 28* |
| 4 | 75 | 88 | 0* |
| H,L= | 5, | 7 | |
| 1 | 73 | 79 | 21* |
| 2 | 0 | 69 | -74* |
| 3 | 70 | 83 | 64* |
| H,L= | 5, | 8 | |
| 0 | 76 | 64 | 17 |
| 1 | 56 | 78 | -3* |
| 2 | 93 | 73 | 14 |
| H,L= | 6, | -12 | |
| 0 | 275 | 48 | -25 |
| 1 | 169 | 22 | 20 |

STRUCTURE FACTORS CONTINUED FOR
THE NORBORNANE DERIVATIVE [ C9 H14 O3 ].

| K | FOB | SG | DEL |
|---|---|---|---|
| 2 | 61 | 75 | 28* |
| H,L= | 6, | -11 | |
| 1 | 84 | 89 | -16* |
| 2 | 97 | 115 | -25* |
| 3 | 35 | 78 | -14* |
| H,L= | 6, | -10 | |
| 0 | 66 | 27 | 18 |
| 1 | 81 | 27 | 53 |
| 2 | 69 | 82 | 67* |
| 3 | 35 | 58 | 2* |
| 4 | 73 | 86 | -35* |
| H,L= | 6, | -9 | |
| 1 | 93 | 30 | -2 |
| 2 | 73 | 74 | 15* |
| 3 | 74 | 96 | -3* |
| 4 | 210 | 9 | 8 |
| 5 | 203 | 10 | 24 |
| H,L= | 6, | -8 | |
| 0 | 43 | 69 | 25* |
| 1 | 323 | 7 | 4 |
| 2 | 435 | 13 | -3 |
| 3 | 450 | 14 | -9 |
| 4 | 149 | 17 | 28 |
| 5 | 150 | 18 | 14 |
| H,L= | 6, | -7 | |
| 1 | 436 | 12 | -3 |
| 2 | 12 | 53 | -15* |
| 3 | 68 | 83 | 31* |
| 4 | 17 | 63 | 14* |
| 5 | 0 | 78 | -4* |
| H,L= | 6, | -6 | |
| 0 | 487 | 6 | 2 |
| 1 | 319 | 12 | 16 |
| 2 | 626 | 8 | 6 |
| 3 | 54 | 60 | 13* |
| 4 | 104 | 29 | -15 |
| 5 | 57 | 70 | 1* |
| 6 | 42 | 73 | 35* |
| H,L= | 6, | -5 | |
| 1 | 43 | 49 | 41* |
| 2 | 320 | 12 | 2 |
| 3 | 218 | 46 | 22 |
| 4 | 341 | 8 | 7 |
| 5 | 109 | 16 | -18 |
| 6 | 180 | 17 | 6 |
| H,L= | 6, | -4 | |
| 0 | 43 | 62 | -8* |
| 1 | 611 | 8 | 4 |
| 2 | 121 | 17 | -12 |
| 3 | 192 | 8 | 4 |
| 4 | 260 | 11 | -12 |
| 5 | 70 | 43 | -13 |
| 6 | 84 | 104 | 12* |
| H,L= | 6, | -3 | |
| 1 | 150 | 19 | 0 |
| 2 | 366 | 6 | 8 |
| 3 | 357 | 7 | 4 |

| K | FOB | SG | DEL |
|---|---|---|---|
| 4 | 372 | 14 | 8 |
| 5 | 66 | 93 | -10* |
| 6 | 127 | 22 | -41 |
| H,L= | 6, | -2 | |
| 0 | 210 | 21 | -5 |
| 1 | 302 | 6 | 2 |
| 2 | 106 | 11 | 16 |
| 3 | 437 | 6 | -5 |
| 4 | 312 | 16 | -6 |
| 5 | 55 | 70 | 7* |
| 6 | 53 | 64 | -2* |
| H,L= | 6, | -1 | |
| 1 | 308 | 7 | -1 |
| 2 | 41 | 48 | -10* |
| 3 | 355 | 8 | -10 |
| 4 | 158 | 13 | 10 |
| 5 | 194 | 12 | 1 |
| 6 | 110 | 15 | 84 |
| H,L= | 6, | 0 | |
| 0 | 599 | 7 | 6 |
| 1 | 117 | 26 | 24 |
| 2 | 255 | 9 | 14 |
| 3 | 129 | 16 | 16 |
| 4 | 222 | 16 | -20 |
| 5 | 33 | 59 | 28* |
| 6 | 106 | 35 | -12 |
| H,L= | 6, | 1 | |
| 1 | 110 | 36 | 6 |
| 2 | 131 | 19 | 2 |
| 3 | 122 | 19 | -23 |
| 4 | 286 | 14 | -5 |
| 5 | 98 | 50 | -10 |
| 6 | 138 | 40 | 30 |
| H,L= | 6, | 2 | |
| 0 | 259 | 8 | 2 |
| 1 | 461 | 11 | 10 |
| 2 | 277 | 6 | 8 |
| 3 | 397 | 16 | 14 |
| 4 | 32 | 70 | 29* |
| 5 | 47 | 63 | 15* |
| H,L= | 6, | 3 | |
| 1 | 349 | 12 | -5 |
| 2 | 204 | 29 | -19 |
| 3 | 127 | 22 | 45 |
| 4 | 45 | 63 | -61* |
| 5 | 0 | 61 | -10* |
| H,L= | 6, | 4 | |
| 0 | 168 | 12 | -6 |
| 1 | 773 | 13 | 5 |
| 2 | 79 | 84 | -3* |
| 3 | 249 | 12 | -3 |
| 4 | 0 | 75 | -47* |
| H,L= | 6, | 5 | |
| 1 | 141 | 36 | -33 |
| 2 | 59 | 70 | -6* |
| 3 | 85 | 102 | 83* |
| 4 | 91 | 109 | 85* |

| K | FOB | SG | DEL |
|---|---|---|---|
| H,L= | 6, | 6 | |
| 0 | 183 | 19 | -7 |
| 1 | 160 | 27 | -46 |
| 2 | 130 | 27 | 3 |
| 3 | 58 | 73 | 38* |
| H,L= | 6, | 7 | |
| 1 | 132 | 18 | 2 |
| 2 | 101 | 16 | 72 |
| H,L= | 7, | -12 | |
| 0 | 271 | 22 | -1 |
| 1 | 89 | 22 | 77 |
| 2 | 98 | 49 | 47 |
| H,L= | 7, | -11 | |
| 1 | 123 | 28 | -6 |
| 2 | 212 | 14 | -31 |
| 3 | 134 | 32 | -23 |
| H,L= | 7, | -10 | |
| 0 | 100 | 42 | 14 |
| 1 | 223 | 9 | -8 |
| 2 | 41 | 97 | 20* |
| 3 | 124 | 19 | 16 |
| 4 | 99 | 22 | -11 |
| H,L= | 7, | -9 | |
| 1 | 244 | 12 | 10 |
| 2 | 187 | 29 | -24 |
| 3 | 0 | 66 | -16* |
| 4 | 234 | 39 | -2 |
| H,L= | 7, | -8 | |
| 0 | 426 | 11 | -6 |
| 1 | 90 | 44 | 2 |
| 2 | 145 | 41 | 9 |
| 3 | 185 | 16 | -8 |
| 4 | 9 | 90 | -9* |
| 5 | 48 | 63 | 38* |
| H,L= | 7, | -7 | |
| 1 | 0 | 52 | -26* |
| 2 | 72 | 26 | 50 |
| 3 | 70 | 42 | 64 |
| 4 | 282 | 19 | 7 |
| 5 | 36 | 60 | 26* |
| H,L= | 7, | -6 | |
| 0 | 79 | 33 | 28 |
| 1 | 150 | 17 | 33 |
| 2 | 35 | 64 | -1* |
| 3 | 66 | 49 | 17 |
| 4 | 109 | 76 | 2 |
| 5 | 73 | 87 | 3* |
| H,L= | 7, | -5 | |
| 1 | 30 | 50 | -29* |
| 2 | 54 | 64 | 41* |
| 3 | 113 | 23 | 6 |
| 4 | 79 | 65 | -20 |
| 5 | 105 | 36 | 31 |
| 6 | 34 | 68 | -14* |
| H,L= | 7, | -4 | |
| 0 | 156 | 16 | -25 |
| 1 | 82 | 22 | 11 |

| K | FOB | SG | DEL |
|---|---|---|---|
| 2 | 103 | 31 | -31 |
| 3 | 79 | 47 | 57 |
| 4 | 101 | 42 | -10 |
| 5 | 84 | 99 | 22* |
| 6 | 167 | 12 | 12 |
| H,L= | 7, | -3 | |
| 1 | 161 | 31 | 8 |
| 2 | 416 | 7 | -9 |
| 3 | 156 | 26 | 6 |
| 4 | 245 | 13 | -1 |
| 5 | 70 | 98 | 58* |
| 6 | 66 | 89 | -40* |
| H,L= | 7, | -2 | |
| 0 | 200 | 20 | 3 |
| 1 | 277 | 11 | -3 |
| 2 | 89 | 50 | -11 |
| 3 | 256 | 15 | -4 |
| 4 | 292 | 24 | 10 |
| 5 | 79 | 93 | 65* |
| 6 | 72 | 76 | 28* |
| H,L= | 7, | -1 | |
| 1 | 180 | 14 | 2 |
| 2 | 32 | 54 | 31* |
| 3 | 291 | 9 | -17 |
| 4 | 344 | 21 | 1 |
| 5 | 108 | 28 | 74 |
| 6 | 150 | 20 | 18 |
| H,L= | 7, | 0 | |
| 0 | 124 | 15 | 0 |
| 1 | 72 | 74 | -18* |
| 2 | 139 | 12 | -1 |
| 3 | 205 | 14 | -16 |
| 4 | 185 | 39 | 1 |
| 5 | 71 | 84 | 68* |
| H,L= | 7, | 1 | |
| 1 | 88 | 20 | -6 |
| 2 | 0 | 68 | -51* |
| 3 | 228 | 27 | 9 |
| 4 | 82 | 96 | -9* |
| 5 | 192 | 27 | 21 |
| H,L= | 7, | 2 | |
| 0 | 114 | 60 | 16 |
| 1 | 74 | 88 | 9* |
| 2 | 70 | 83 | -15* |
| 3 | 316 | 16 | 1 |
| 4 | 130 | 22 | -15 |
| 5 | 142 | 59 | 29 |
| H,L= | 7, | 3 | |
| 1 | 129 | 24 | 12 |
| 2 | 0 | 68 | -13* |
| 3 | 150 | 27 | 3 |
| 4 | 18 | 60 | -70* |
| H,L= | 7, | 4 | |
| 0 | 266 | 13 | 1 |
| 1 | 57 | 74 | -44* |
| 2 | 148 | 13 | 5 |
| 3 | 0 | 58 | -41* |

| K | FOB | SG | DEL |
|---|---|---|---|
| 4 | 108 | 29 | 19 |
| H,L= | 7, | 5 | |
| 1 | 123 | 40 | 12 |
| 2 | 50 | 90 | 42* |
| 3 | 62 | 74 | 51* |
| H,L= | 7, | 6 | |
| 0 | 226 | 8 | 17 |
| 1 | 67 | 44 | 30 |
| 2 | 22 | 63 | 18* |
| H,L= | 8, | -12 | |
| 0 | 111 | 51 | 6 |
| 1 | 155 | 61 | -7 |
| H,L= | 8, | -11 | |
| 1 | 69 | 51 | 25 |
| 2 | 83 | 40 | 48 |
| 3 | 74 | 88 | 40* |
| H,L= | 8, | -10 | |
| 0 | 230 | 23 | 13 |
| 1 | 141 | 22 | 4 |
| 2 | 31 | 56 | 18* |
| 3 | 216 | 39 | 4 |
| H,L= | 8, | -9 | |
| 1 | 358 | 8 | -10 |
| 2 | 260 | 17 | -13 |
| 3 | 196 | 21 | -8 |
| 4 | 0 | 60 | -50* |
| H,L= | 8, | -8 | |
| 0 | 423 | 8 | 18 |
| 1 | 233 | 20 | -10 |
| 2 | 207 | 30 | -17 |
| 3 | 146 | 32 | -5 |
| 4 | 202 | 10 | 13 |
| H,L= | 8, | -7 | |
| 1 | 247 | 10 | -1 |
| 2 | 78 | 41 | -1 |
| 3 | 89 | 98 | -33* |
| 4 | 367 | 8 | -3 |
| 5 | 99 | 25 | 6 |
| H,L= | 8, | -6 | |
| 0 | 34 | 58 | 18* |
| 1 | 218 | 23 | 8 |
| 2 | 0 | 87 | -14* |
| 3 | 320 | 10 | -12 |
| 4 | 89 | 97 | -7* |
| 5 | 162 | 17 | -3 |
| H,L= | 8, | -5 | |
| 1 | 0 | 64 | -33* |
| 2 | 181 | 14 | -6 |
| 3 | 199 | 20 | -10 |
| 4 | 204 | 24 | 5 |
| 5 | 119 | 17 | -3 |
| H,L= | 8, | -4 | |
| 0 | 386 | 31 | 3 |
| 1 | 249 | 14 | -1 |
| 2 | 86 | 103 | 21* |
| 3 | 115 | 44 | 5 |
| 4 | 290 | 10 | -7 |

STRUCTURE FACTORS CONTINUED FOR
THE NORBORNANE DERIVATIVE [ C9 H14 O3 ].

| K | FOB | SG | DEL |
|---|---|---|---|
| 5 | 69 | 42 | 37 |
| H,L= | 8, | -3 | |
| 1 | 51 | 67 | -27* |
| 2 | 141 | 11 | -4 |
| 3 | 403 | 9 | -18 |
| 4 | 13 | 79 | -19* |
| 5 | 59 | 73 | 40* |
| H,L= | 8, | -2 | |
| 0 | 109 | 21 | -20 |
| 1 | 530 | 9 | -7 |
| 2 | 0 | 54 | -35* |
| 3 | 261 | 18 | 2 |
| 4 | 296 | 11 | 18 |
| 5 | 209 | 25 | -17 |
| H,L= | 8, | -1 | |
| 1 | 199 | 21 | -11 |
| 2 | 78 | 43 | 18 |
| 3 | 348 | 9 | -3 |
| 4 | 134 | 33 | 8 |
| 5 | 0 | 62 | -20* |
| H,L= | 8, | 0 | |
| 0 | 46 | 66 | 18* |
| 1 | 36 | 56 | -21* |
| 2 | 146 | 18 | 5 |
| 3 | 311 | 11 | -1 |
| 4 | 170 | 56 | 9 |
| 5 | 114 | 29 | 21 |
| H,L= | 8, | 1 | |
| 1 | 238 | 7 | 10 |
| 2 | 204 | 20 | 16 |
| 3 | 115 | 14 | 1 |
| 4 | 70 | 83 | 48* |
| H,L= | 8, | 2 | |
| 0 | 290 | 11 | -23 |
| 1 | 118 | 26 | 17 |
| 2 | 112 | 15 | 8 |
| 3 | 66 | 32 | -10 |
| 4 | 39 | 87 | 14* |
| H,L= | 8, | 3 | |
| 1 | 127 | 28 | 1 |
| 2 | 96 | 34 | 62 |
| 3 | 68 | 90 | 50* |
| H,L= | 8, | 4 | |
| 0 | 0 | 58 | -41* |
| 1 | 35 | 58 | -35* |
| 2 | 125 | 26 | 14 |
| 3 | 151 | 36 | 48 |
| H,L= | 8, | 5 | |
| 1 | 31 | 72 | -51* |
| H,L= | 9, | -12 | |
| 0 | 61 | 73 | -11* |
| H,L= | 9, | -11 | |
| 1 | 115 | 42 | 18 |
| 2 | 178 | 25 | -6 |
| H,L= | 9, | -10 | |
| 0 | 207 | 20 | 15 |
| 1 | 152 | 24 | 37 |
| 2 | 35 | 67 | -43* |
| 3 | 0 | 61 | -41* |
| H,L= | 9, | -9 | |
| 1 | 105 | 30 | -23 |
| 2 | 54 | 65 | 30* |
| 3 | 67 | 80 | 29* |
| 4 | 130 | 39 | -11 |
| H,L= | 9, | -8 | |
| 0 | 35 | 89 | 30* |
| 1 | 213 | 8 | 9 |
| 2 | 73 | 44 | 21 |
| 3 | 79101 | | 8* |
| 4 | 65107 | | 56* |
| H,L= | 9, | -7 | |
| 1 | 98 | 23 | -19 |
| 2 | 80 | 48 | 13 |
| 3 | 116 | 21 | -9 |
| 4 | 69 | 82 | -7* |
| H,L= | 9, | -6 | |
| 0 | 122 | 26 | -13 |
| 1 | 149 | 26 | -5 |
| 2 | 54 | 64 | 23* |
| 3 | 157 | 26 | 14 |
| 4 | 0 | 78 | -39* |
| H,L= | 9, | -5 | |
| 1 | 63 | 99 | 14* |
| 2 | 48 | 72 | 39* |
| 3 | 161 | 16 | -1 |
| 4 | 107 | 19 | 8 |
| 5 | 105 | 91 | -11 |
| H,L= | 9, | -4 | |
| 0 | 181 | 19 | -10 |
| 1 | 336 | 7 | 2 |
| 2 | 107107 | | -27* |
| 3 | 186 | 23 | -19 |
| 4 | 194 | 22 | 26 |
| 5 | 0 | 73 | -2* |
| H,L= | 9, | -3 | |
| 1 | 132 | 32 | 12 |
| 2 | 21 | 87 | -34* |
| 3 | 170 | 18 | 3 |
| 4 | 112 | 84 | 18 |
| 5 | 62 | 74 | 18* |
| H,L= | 9, | -2 | |
| 0 | 134 | 20 | 4 |
| 1 | 270 | 11 | -10 |
| 2 | 79 | 94 | -30* |
| 3 | 0 | 62 | -32* |
| 4 | 152 | 40 | 2 |
| H,L= | 9, | -1 | |
| 1 | 89 | 36 | -16 |
| 2 | 53 | 72 | 52* |
| 3 | 151 | 22 | -20 |
| 4 | 66 | 84 | 4* |
| H,L= | 9, | 0 | |
| 0 | 175 | 21 | -10 |
| 1 | 59 | 64 | 32* |
| 2 | 319 | 21 | -13 |
| 3 | 194 | 20 | 2 |
| 4 | 37 | 59 | -29* |
| H,L= | 9, | 1 | |
| 1 | 53 | 57 | 42* |
| 2 | 267 | 9 | 0 |
| 3 | 79 | 98 | -9* |
| 4 | 28 | 80 | 25* |
| H,L= | 9, | 2 | |
| 0 | 217 | 9 | 1 |
| 1 | 230 | 21 | 38 |
| 2 | 0109 | | -57* |
| 3 | 91 | 27 | 55 |
| H,L= | 9, | 3 | |
| 1 | 62 | 80 | 29* |
| 2 | 94 | 82 | 26 |
| H,L= | 9, | 4 | |
| 0 | 93 | 24 | -22 |
| 1 | 113 | 30 | 15 |
| H,L= | 10, | -11 | |
| 1 | 96 | 29 | -11 |
| H,L= | 10, | -10 | |
| 0 | 351 | 15 | -5 |
| 1 | 207 | 18 | 15 |
| 2 | 30 | 72 | -9* |
| H,L= | 10, | -9 | |
| 1 | 322 | 17 | 2 |
| 2 | 0 | 58 | -2* |
| 3 | 132 | 33 | 4 |
| H,L= | 10, | -8 | |
| 0 | 302 | 18 | -7 |
| 1 | 214 | 17 | -10 |
| 2 | 0 | 88 | -11* |
| 3 | 82 | 69 | 5 |
| H,L= | 10, | -7 | |
| 1 | 86 | 42 | 53 |
| 2 | 165 | 34 | 22 |
| 3 | 26 | 84 | 10* |
| 4 | 66 | 85 | 30* |
| H,L= | 10, | -6 | |
| 0 | 296 | 15 | 3 |
| 1 | 325 | 16 | 5 |
| 2 | 226 | 30 | -3 |
| 3 | 119 | 28 | -33 |
| 4 | 246 | 19 | -3 |
| H,L= | 10, | -5 | |
| 1 | 0 | 87 | -29* |
| 2 | 87 | 94 | 27* |
| 3 | 217 | 9 | 3 |
| 4 | 36 | 61 | -36* |
| H,L= | 10, | -4 | |
| 0 | 250 | 12 | 0 |
| 1 | 218 | 15 | 24 |
| 2 | 95 | 30 | 39 |
| 3 | 89105 | | 16* |
| 4 | 139 | 43 | -13 |
| H,L= | 10, | -3 | |
| 1 | 96 | 86 | 22 |
| 2 | 98117 | | 20* |
| 3 | 225 | 11 | -12 |
| 4 | 64 | 77 | 64* |
| H,L= | 10, | -2 | |
| 0 | 158 | 11 | -1 |
| 1 | 321 | 8 | -2 |
| 2 | 167 | 17 | 19 |
| 3 | 140 | 18 | 35 |
| 4 | 58 | 88 | 28* |
| H,L= | 10, | -1 | |
| 1 | 67 | 31 | -2 |
| 2 | 158 | 18 | -4 |
| 3 | 78 | 85 | -54* |
| H,L= | 10, | 0 | |
| 0 | 156 | 14 | -4 |
| 1 | 450 | 17 | -8 |
| 2 | 181 | 14 | -15 |
| 3 | 133 | 15 | -14 |
| H,L= | 10, | 1 | |
| 1 | 193 | 15 | -0 |
| 2 | 58 | 69 | 16* |
| H,L= | 10, | 2 | |
| 0 | 141 | 18 | 33 |
| 1 | 51 | 93 | -19* |
| H,L= | 11, | -10 | |
| 0 | 111 | 19 | -5 |
| 1 | 12 | 87 | -46* |
| H,L= | 11, | -9 | |
| 1 | 91109 | | 24* |
| 2 | 64 | 77 | 28* |
| H,L= | 11, | -8 | |
| 0 | 112 | 28 | 10 |
| 1 | 254 | 27 | -14 |
| 2 | 72 | 85 | 45* |
| H,L= | 11, | -7 | |
| 1 | 35 | 91 | 30* |
| 2 | 296 | 37 | -35 |
| 3 | 108115 | | -1* |
| H,L= | 11, | -6 | |
| 0 | 104 | 33 | 1 |
| 1 | 475 | 12 | -13 |
| 2 | 117 | 49 | 23 |
| 3 | 101 | 31 | 16 |
| H,L= | 11, | -5 | |
| 1 | 85 | 31 | -23 |
| 2 | 85100 | | -6* |
| 3 | 36 | 68 | 15* |
| H,L= | 11, | -4 | |
| 0 | 53 | 63 | 8* |
| 1 | 99 | 30 | 1 |
| 2 | 37 | 73 | -51* |
| 3 | 49 | 67 | 19* |
| H,L= | 11, | -3 | |
| 1 | 99 | 46 | 6 |
| 2 | 30 | 96 | -8* |
| 3 | 48 | 70 | -5* |
| H,L= | 11, | -2 | |
| 0 | 76 | 81 | 11* |
| 1 | 192 | 30 | -0 |
| 2 | 246 | 35 | 11 |
| 3 | 109 | 32 | 30 |
| H,L= | 11, | -1 | |
| 1 | 151 | 39 | 8 |
| 2 | 185 | 15 | -0 |
| H,L= | 11, | 0 | |
| 0 | 123 | 93 | 10 |
| 1 | 224 | 15 | 12 |
| H,L= | 12, | -8 | |
| 0 | 74 | 75 | 40* |
| 1 | 88104 | | 20* |
| H,L= | 12, | -7 | |
| 1 | 13 | 82 | 9* |
| H,L= | 12, | -6 | |
| 0 | 110 | 28 | 40 |
| 1 | 46 | 78 | -14* |
| 2 | 116 | 68 | 19 |
| H,L= | 12, | -5 | |
| 1 | 113 | 48 | -8 |
| 2 | 63 | 91 | -0* |
| H,L= | 12, | -4 | |
| 0 | 51 | 62 | 9* |
| 1 | 64 | 76 | 3* |
| H,L= | 12, | -3 | |
| 1 | 114 | 62 | 28 |

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