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# Intramolecular hydrogen bonding In norbornyl systems.

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TABLE 4. Selected angles (degrees) between bonded atoms of bicyclo[2.2.1]heptane, (66).

| | |
|---|---|
| C(1)-C(2)-C(3) | 102.93 |
| C(2)-C(1)-C(6) | 108.35 |
| C(3)-C(4)-C(5) | 108.35 |
| C(1)-C(7)-C(4) | 93.31 |
| C(2)-C(1)-C(7) | 102.03 |
| H(1)-C(1)-C(7) | 116.23 |
| H(2x)-C(2)-C(3) | 111.74 |
| H(2x)-C(2)-H(2n) | 103.74 |

TABLE 5. Selected dihedral angles (degrees) for bicyclo[2.2.1]heptane, (66).

| | |
|---|---|
| C(1)-C(2)-C(3)-C(4) | 0.00 |
| C(1)-C(6)-C(5)-C(4) | 0.00 |
| H(1)-C(1)-C(7)-H(7a) | -61.30 |
| H(1)-C(1)-C(2)-H(2x) | -41.80 |
| H(3n)-C(3)-C(4)-C(5) | 52.40 |
| H(2x)-C(2)-C(3)-H(3x) | 0.00 |

TABLE 6. Orthogonalised atomic coordinates for 2-exo-nitrobicyclo[2.2.1]heptane, (80).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.964200 | 4.138300 | 3.371800 |
| 2 | C(5) | 1.316203 | 3.343900 | 2.091300 |
| 3 | C(6) | -0.065896 | 2.835462 | 1.612100 |
| 4 | C(1) | -1.036934 | 3.418424 | 2.667578 |
| 5 | C(2) | -0.852179 | 2.647674 | 3.998730 |
| 6 | C(3) | 0.547662 | 3.131274 | 4.470888 |
| 7 | C(7) | -0.385432 | 4.776998 | 2.991377 |
| 8 | H(4) | 1.756996 | 4.828614 | 3.685005 |
| 9 | H(5x) | 1.792553 | 3.991477 | 1.345291 |
| 10 | H(5n) | 2.054038 | 2.550701 | 2.254647 |
| 11 | H(6x) | -0.305515 | 3.203225 | 0.606975 |
| 12 | H(6n) | -0.132961 | 1.746615 | 1.511820 |
| 13 | H(1) | -2.077360 | 3.452893 | 2.323641 |
| 14 | N | -1.935886 | 3.036046 | 4.938296 |
| 15 | H(2n) | -0.896940 | 1.560093 | 3.869302 |
| 16 | H(3x) | 0.549094 | 3.607105 | 5.456621 |
| 17 | H(3n) | 1.273129 | 2.320841 | 4.603269 |
| 18 | H(7s) | -0.866645 | 5.333112 | 3.803602 |
| 19 | H(7a) | -0.335798 | 5.467826 | 2.142152 |
| 20 | O(1) | -1.725393 | 3.647467 | 5.997928 |
| 21 | O(2) | -3.099743 | 2.687918 | 4.683866 |

TABLE 7. Bond lengths (angstrom) for 2-exo-nitrobicyclo[2.2.1]heptane, (80).

| | |
|---|---|
| C(4)-C(5) | 1.5475 |
| C(4)-C(3) | 1.5478 |
| C(4)-C(7) | 1.5408 |
| C(4)-H(4) | 1.0969 |
| C(5)-C(6) | 1.5487 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(6)-C(1) | 1.5482 |
| C(6)-H(6x) | 1.0968 |
| C(6)-H(6n) | 1.0955 |
| C(1)-C(2) | 1.5492 |
| C(1)-C(7) | 1.5411 |
| C(1)-H(1) | 1.0963 |
| C(2)-C(3) | 1.5545 |
| C(2)-N | 1.4859 |
| C(2)-H(2n) | 1.0962 |
| C(3)-H(3x) | 1.0946 |
| C(3)-H(3n) | 1.0957 |
| C(7)-H(7a) | 1.0959 |
| C(7)-H(7s) | 1.0957 |
| N-O(1) | 1.2414 |
| N-O(2) | 1.2412 |

TABLE 8. Selected angles (degrees) between bonded atoms of 2-exo-nitrobicyclo[2.2.1]heptane, (80).

| | |
|---|---|
| O(1)-N-O(2) | 118.17 |
| C(2)-N-O(2) | 118.75 |
| C(2)-N-O(1) | 123.01 |
| H(2n)-C(2)-N | 107.71 |
| C(1)-C(2)-N | 109.04 |
| C(3)-C(2)-N | 112.54 |
| C(1)-C(7)-C(4) | 93.25 |
| C(3)-C(4)-C(5) | 108.35 |
| C(2)-C(1)-C(6) | 108.88 |
| H(1)-C(1)-C(7) | 116.06 |
| H(4)-C(4)-C(7) | 116.28 |

TABLE 9. Selected dihedral angles (degrees) for 2-exo-nitrobicyclo[2.2.1]heptane, (80).

| | |
|---|---|
| C(3)-C(2)-N-O(1) | -1.80 |
| C(3)-C(2)-N-O(2) | -178.80 |
| C(1)-C(2)-N-O(1) | -114.70 |
| C(1)-C(2)-N-O(2) | 68.40 |
| H(2n)-C(2)-N-O(1) | 122.60 |
| C(1)-C(2)-C(3)-C(4) | 1.40 |
| C(1)-C(6)-C(5)-C(4) | 0.70 |
| H(1)-C(1)-C(7)-H(7s) | 62.00 |
| H(4)-C(4)-C(7)-H(7s) | -61.00 |
| H(3x)-C(3)-C(2)-N | 4.90 |

TABLE 10. Orthogonalised atomic coordinates for 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(4) | -0.318145 | 2.576712 | 5.367439 |
| 3 | C(5) | 0.798587 | 0.789594 | 6.074071 |
| 4 | H(5x) | 0.277712 | 0.160312 | 5.342272 |
| 5 | H(5n) | 0.316377 | 0.535639 | 0.535639 |
| 6 | C(6) | 2.328866 | 0.553699 | 6.054602 |

| | | | | |
|---|---|---|---|---|
| 7 | H(6n) | 2.728377 | 0.155877 | 6.993038 |
| 8 | H(6x) | 2.605819 | -0.213332 | 5.321147 |
| 9 | C(1) | 2.898077 | 1.936322 | 5.648359 |
| 10 | H(1) | 3.920144 | 1.888298 | 5.253903 |
| 11 | C(2) | 2.746786 | 2.943689 | 6.817513 |
| 12 | H(2x) | 3.258562 | 3.887640 | 6.590642 |
| 13 | N | 3.307747 | 2.400965 | 8.076872 |
| 14 | O(1) | 4.439207 | 1.890814 | 8.044907 |
| 15 | O(2) | 2.938595 | 2.894553 | 9.154450 |
| 16 | C(3) | 1.206768 | 3.120865 | 6.896864 |
| 17 | H(3x) | 0.925085 | 4.175808 | 6.796840 |
| 18 | H(3n) | 0.752427 | 2.831551 | 7.850175 |
| 19 | C(7) | 1.819780 | 2.443228 | 4.669806 |
| 20 | H(7s) | 1.968407 | 3.469860 | 4.316450 |
| 21 | H(7a) | 1.701682 | 1.830895 | 3.768659 |

TABLE 11. Bond lengths (angstrom) for 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | |
|---|---|
| C(4)-H(4) | 1.0968 |
| C(4)-C(5) | 1.5467 |
| C(3)-C(4) | 1.5482 |
| C(4)-C(7) | 1.5413 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(5)-C(6) | 1.5485 |
| C(6)-H(6n) | 1.0948 |
| C(6)-H(6x) | 1.0968 |
| C(6)-C(1) | 1.5494 |
| C(1)-H(1) | 1.0966 |
| C(1)-C(2) | 1.5507 |
| C(1)-C(7) | 1.5418 |
| C(2)-H(2x) | 1.0975 |
| C(2)-N | 1.4816 |
| C(2)-C(3) | 1.5522 |
| N-O(1) | 1.2414 |
| N-O(2) | 1.2416 |
| C(3)-H(3x) | 1.0965 |
| C(3)-H(3n) | 1.0950 |
| C(7)-H(7s) | 1.0959 |
| C(7)-H(7a) | 1.0959 |

TABLE 12. Selected angles (degrees) between bonded atoms of 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | |
|---|---|
| C(1)-C(2)-C(3) | 102.09 |
| C(1)-C(2)-H(2x) | 110.94 |
| C(3)-C(2)-H(2x) | 112.03 |
| C(1)-C(7)-C(4) | 93.24 |
| C(2)-C(1)-C(6) | 108.12 |
| C(3)-C(4)-C(5) | 110.25 |
| C(1)-C(2)-N | 111.47 |
| C(3)-C(2)-N | 111.96 |
| O(1)-N-O(2) | 117.18 |
| C(2)-N-O(2) | 118.27 |

| | | | | |
|---|---|---|---|---|
| 7 | H(6n) | 2.728377 | 0.155877 | 6.993038 |
| 8 | H(6x) | 2.605819 | -0.213332 | 5.321147 |
| 9 | C(1) | 2.898077 | 1.936322 | 5.648359 |
| 10 | H(1) | 3.920144 | 1.888298 | 5.253903 |
| 11 | C(2) | 2.746786 | 2.943689 | 6.817513 |
| 12 | H(2x) | 3.258562 | 3.887640 | 6.590642 |
| 13 | N | 3.307747 | 2.400965 | 8.076872 |
| 14 | O(1) | 4.439207 | 1.890814 | 8.044907 |
| 15 | O(2) | 2.938595 | 2.894553 | 9.154450 |
| 16 | C(3) | 1.206768 | 3.120865 | 6.896864 |
| 17 | H(3x) | 0.925085 | 4.175808 | 6.796840 |
| 18 | H(3n) | 0.752427 | 2.831551 | 7.850175 |
| 19 | C(7) | 1.819780 | 2.443228 | 4.669806 |
| 20 | H(7s) | 1.968407 | 3.469860 | 4.316450 |
| 21 | H(7a) | 1.701682 | 1.830895 | 3.768659 |

TABLE 11. Bond lengths (angstrom) for 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | |
|---|---|
| C(4)-H(4) | 1.0968 |
| C(4)-C(5) | 1.5467 |
| C(3)-C(4) | 1.5482 |
| C(4)-C(7) | 1.5413 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(5)-C(6) | 1.5485 |
| C(6)-H(6n) | 1.0948 |
| C(6)-H(6x) | 1.0968 |
| C(6)-C(1) | 1.5494 |
| C(1)-H(1) | 1.0966 |
| C(1)-C(2) | 1.5507 |
| C(1)-C(7) | 1.5418 |
| C(2)-H(2x) | 1.0975 |
| C(2)-N | 1.4816 |
| C(2)-C(3) | 1.5522 |
| N-O(1) | 1.2414 |
| N-O(2) | 1.2416 |
| C(3)-H(3x) | 1.0965 |
| C(3)-H(3n) | 1.0950 |
| C(7)-H(7s) | 1.0959 |
| C(7)-H(7a) | 1.0959 |

TABLE 12. Selected angles (degrees) between bonded atoms of 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | |
|---|---|
| C(1)-C(2)-C(3) | 102.09 |
| C(1)-C(2)-H(2x) | 110.94 |
| C(3)-C(2)-H(2x) | 112.03 |
| C(1)-C(7)-C(4) | 93.24 |
| C(2)-C(1)-C(6) | 108.12 |
| C(3)-C(4)-C(5) | 110.25 |
| C(1)-C(2)-N | 111.47 |
| C(3)-C(2)-N | 111.96 |
| O(1)-N-O(2) | 117.18 |
| C(2)-N-O(2) | 118.27 |

TABLE 13. Selected dihedral angles (degrees) for 2-endo-nitrobicyclo[2.2.1]heptane, (69).

| | |
|---|---|
| C(3)-C(2)-N-O(1) | -46.10 |
| H(2X)-C(2)-N-O(1) | 77.90 |
| C(1)-C(2)-C(3)-C(4) | -4.30 |
| C(4)-C(5)-C(6)-C(1) | -1.00 |
| C(6)-C(1)-C(2)-N | 52.00 |
| H(2X)-C(2)-C(3)-H(3X) | -4.90 |
| H(3X)-C(3)-C(4)-H(4) | 42.80 |
| H(1)-C(1)-C(7)-H(7a) | -61.90 |
| H(4)-C(4)-C(7)-H(7a) | 60.40 |

TABLE 14. Orthogonalised atomic coordinates for 2-exo-chloro-2-endo-nitrobicyclo[2.2.1]heptane, (71).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(4) | -0.318359 | 2.576712 | 5.367439 |
| 3 | C(5) | 0.791733 | 0.788777 | 6.074071 |
| 4 | H(5x) | 0.239030 | 0.159885 | 5.365674 |
| 5 | H(5n) | 0.338787 | 0.548350 | 7.042224 |
| 6 | C(6) | 2.316998 | 0.531659 | 6.005023 |
| 7 | H(6n) | 2.730622 | 0.073876 | 6.909263 |
| 8 | H(6x) | 2.561770 | -0.205054 | 5.229843 |
| 9 | C(1) | 2.898121 | 1.922070 | 5.641849 |
| 10 | H(1) | 3.916533 | 1.851097 | 5.240213 |
| 11 | C(2) | 2.747299 | 2.883109 | 6.854162 |
| 12 | Cl | 3.632952 | 4.386615 | 6.575246 |
| 13 | N | 3.245815 | 2.260515 | 8.104160 |
| 14 | O(1) | 4.361935 | 1.716354 | 8.088346 |
| 15 | O(2) | 2.845679 | 2.699956 | 9.194192 |
| 16 | C(3) | 1.209931 | 3.124782 | 6.893320 |
| 17 | H(3x) | 0.906036 | 4.172264 | 6.778946 |
| 18 | H(3n) | 0.731102 | 2.854453 | 7.839964 |
| 19 | C(7) | 1.818580 | 2.440918 | 4.668532 |
| 20 | H(7s) | 1.958794 | 3.463549 | 4.302122 |
| 21 | H(7a) | 1.690244 | 1.830846 | 3.767105 |

TABLE 15. Bond lengths (angstrom) for 2-exo-chloro-2-endo-nitrobicyclo[2.2.1]heptane, (71).

| | |
|---|---|
| C(4)-H(4) | 1.0970 |
| C(4)-C(5) | 1.5470 |
| C(4)-C(3) | 1.5486 |
| C(4)-C(7) | 1.5410 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(5)-C(6) | 1.5483 |
| C(6)-H(6x) | 1.0971 |
| C(6)-H(6n) | 1.0947 |
| C(6)-C(1) | 1.5501 |
| C(1)-H(1) | 1.0970 |
| C(1)-C(2) | 1.5544 |
| C(1)-C(7) | 1.5434 |
| C(2)-Cl | 1.7671 |
| C(2)-N | 1.4828 |
| C(2)-C(3) | 1.5567 |
| N-O(1) | 1.2415 |
| N-O(2) | 1.2418 |
| C(3)-H(3x) | 1.0967 |
| C(3)-H(3n) | 1.0948 |
| C(7)-H(7s) | 1.0953 |
| C(7)-H(7a) | 1.0960 |

TABLE 16. Selected angles (degrees) between bonded atoms of 2-exo-chloro-2-endo-nitrobicyclo[2.2.1]heptane, (71).

| | |
|---|---|
| C(1)-C(2)-C(3) | 102.21 |
| C(1)-C(2)-Cl | 110.75 |
| C(3)-C(2)-Cl | 111.52 |
| C(1)-C(7)-C(4) | 93.32 |
| C(2)-C(1)-C(6) | 109.60 |
| C(3)-C(4)-C(5) | 108.39 |
| C(1)-C(2)-N | 111.42 |
| C(3)-C(2)-N | 112.09 |
| O(1)-N-O(2) | 117.13 |
| C(2)-N-O(2) | 118.39 |

TABLE 17. Selected dihedral angles for 2-exo-chloro-2-endo-nitrobicyclo[2.2.1]heptane, (71).

| | |
|---|---|
| C(3)-C(2)-N-O(1) | -44.70 |
| Cl-O(2)-N-O(1) | 79.10 |
| O(1)-O(2)-O(3)-O(4) | -0.40 |
| O(4)-O(5)-O(6)-O(1) | 1.60 |
| O(6)-O(1)-O(2)-N | 49.40 |
| Cl-O(2)-O(3)-H(3x) | -1.90 |
| H(3x)-O(3)-O(4)-H(4) | -38.30 |
| H(1)-O(1)-O(7)-H(7a) | -62.60 |
| H(4)-O(4)-O(7)-H(7a) | 59.60 |

TABLE 18. Orthogonalised atomic coordinates for 6-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (73).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(4) | -0.318308 | 2.576712 | 5.367439 |
| 3 | C(5) | 0.787233 | 0.787499 | 6.074071 |
| 4 | H(5x) | 0.174629 | 0.154031 | 5.421326 |
| 5 | H(5n) | 0.412944 | 0.556578 | 7.076810 |
| 6 | C(6) | 2.297613 | 0.511939 | 5.893505 |
| 7 | O(1) | 2.821724 | -0.265592 | 6.978380 |
| 8 | H | 3.388271 | 0.053281 | 7.653831 |
| 9 | H(6x) | 2.468861 | -0.107006 | 5.003093 |
| 10 | C(1) | 2.908785 | 1.922595 | 5.646498 |
| 11 | H(1) | 3.927572 | 1.859926 | 5.245514 |
| 12 | C(2) | 2.748814 | 2.938095 | 6.818835 |
| 13 | Cl | 3.557635 | 4.482609 | 6.422061 |
| 14 | N | 3.330315 | 2.437552 | 8.085648 |
| 15 | O(1) | 4.532345 | 2.124789 | 8.079282 |
| 16 | O(2) | 2.859984 | 2.832797 | 9.164477 |
| 17 | C(3) | 1.205022 | 3.119826 | 6.899052 |
| 18 | H(3x) | 0.863261 | 4.159006 | 6.823851 |
| 19 | H(3n) | 0.755590 | 2.814418 | 7.849253 |
| 20 | C(7) | 1.825148 | 2.450032 | 4.674415 |
| 21 | H(7s) | 1.946406 | 3.471480 | 4.299010 |
| 22 | H(7a) | 1.687077 | 1.864024 | 3.758312 |

TABLE 19. Bond lengths (angstrom) for 6-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (73).

| | |
|---|---|
| C(4)-H(4) | 1.0970 |
| C(4)-C(3) | 1.5473 |
| C(4)-C(5) | 1.5505 |
| C(4)-C(7) | 1.5421 |
| C(3)-H(3x) | 1.0968 |
| C(3)-H(3n) | 1.0948 |
| C(3)-C(2) | 1.5493 |
| C(2)-O(1) | 1.4341 |
| C(2)-H(2x) | 1.0974 |
| C(2)-C(1) | 1.5552 |
| O(1)-H | 0.9424 |
| C(1)-H(1) | 1.0967 |
| C(1)-C(6) | 1.5559 |
| C(1)-C(7) | 1.5464 |
| C(6)-Cl | 1.7876 |
| C(6)-N | 1.4810 |
| C(6)-C(5) | 1.5560 |
| N-O(2) | 1.2418 |
| N-O(3) | 1.2414 |
| C(5)-H(5x) | 1.0964 |
| C(5)-H(5n) | 1.0947 |
| C(7)-H(7a) | 1.0949 |
| C(7)-H(7s) | 1.0962 |

TABLE 20. Selected angles (degrees) between bonded atoms of 6-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (73).

| | |
|---|---|
| C(1)-C(6)-C(5) | 101.86 |
| C(5)-C(6)-Cl | 111.44 |
| C(1)-C(6)-Cl | 110.67 |
| C(1)-C(6)-N | 112.28 |
| C(5)-C(6)-N | 112.57 |
| O(2)-N-O(3) | 117.20 |
| Cl-C(6)-N | 108.00 |
| C(2)-O(1)-H | 123.23 |
| C(1)-C(2)-O(1) | 115.13 |
| C(3)-C(2)-O(1) | 112.43 |
| C(1)-C(7)-C(4) | 93.41 |
| C(1)-C(2)-C(3) | 104.17 |
| H(2x)-C(2)-O(1) | 115.13 |
| H(1)-C(1)-C(7) | 116.05 |
| C(3)-C(2)-H(2x) | 110.34 |
| C(1)-C(2)-H(2x) | 109.41 |

TABLE 21. Selected dihedral angles (degrees) for 6-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (73).

| | |
|---|---|
| C(5)-C(6)-N-O(3) | -42.30 |
| Cl-C(6)-N-O(3) | 81.10 |
| C(3)-C(2)-O(1)-H | -38.00 |
| H(2x)-C(2)-O(1)-H | -158.20 |
| Cl-C(6)-C(5)-H(5x) | -9.10 |
| N-C(6)-C(1)-C(2) | 56.40 |
| O(1)-C(2)-C(1)-C(6) | -55.80 |
| C(1)-C(2)-C(3)-C(4) | 2.30 |
| C(1)-C(6)-C(5)-C(4) | -6.10 |
| H(1)-C(1)-C(7)-H(7s) | -62.30 |
| H(4)-C(4)-C(7)-H(7s) | 57.20 |

TABLE 22. Selected non-bonded distances (angstrom) for 6-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (73).

| | |
|---|---|
| O(1)...O(2) | 2.864 |
| O(1)...O(3) | 3.622 |
| O(1)...N | 2.767 |
| H...O(2) | 2.776 |
| H...O(3) | 3.060 |
| H...N | 2.493 |

TABLE 23. Orthogonolised atomic coordinates for 6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (72).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(4) | -0.318157 | 2.576712 | 5.367439 |
| 3 | C(5) | 0.802267 | 0.787193 | 6.074071 |
| 4 | H(5x) | 0.186152 | 0.154007 | 5.424631 |
| 5 | H(5n) | 0.433469 | 0.558995 | 7.079542 |
| 6 | C(6) | 2.310923 | 0.499845 | 5.884033 |
| 7 | O(1) | 2.867351 | -0.161671 | 7.026887 |
| 8 | H(6x) | 2.485855 | -0.145934 | 5.012858 |
| 9 | C(1) | 2.900540 | 1.911967 | 5.635633 |
| 10 | H(1) | 3.925494 | 1.883456 | 5.247667 |
| 11 | C(2) | 2.728249 | 2.875698 | 6.841154 |
| 12 | H(2x) | 3.255149 | 3.820257 | 6.653800 |
| 13 | N | 3.269969 | 2.302220 | 8.095822 |
| 14 | O(2) | 4.499670 | 2.189012 | 8.218864 |
| 15 | O(3) | 2.539185 | 1.822058 | 8.977504 |
| 16 | C(3) | 1.196950 | 3.126134 | 6.896374 |
| 17 | H(3x) | 0.955191 | 4.186969 | 6.757480 |
| 18 | H(3n) | 0.697206 | 2.894558 | 7.842209 |
| 19 | C(7) | 1.826084 | 2.472162 | 4.678907 |
| 20 | H(7s) | 1.989483 | 3.509207 | 4.364115 |
| 21 | H(7a) | 1.690524 | 1.909442 | 3.748240 |
| 22 | H | 3.793120 | -0.330042 | 7.096900 |

TABLE 24. Bond lengths (angstrom) of 6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (72).

| | |
|---|---|
| C(4)-H(4) | 1.0968 |
| C(4)-C(3) | 1.5493 |
| C(4)-C(5) | 1.5474 |
| C(4)-C(7) | 1.5431 |
| C(3)-H(3x) | 1.0965 |
| C(3)-H(3n) | 1.0950 |
| C(3)-C(2) | 1.5475 |
| C(2)-O(1) | 1.4329 |
| C(2)-H(2x) | 1.0984 |
| C(2)-C(1) | 1.5503 |
| O(1)-H | 0.9436 |
| C(1)-H(1) | 1.0963 |
| C(1)-C(6) | 1.5530 |
| C(1)-C(7) | 1.5439 |
| C(6)-H(6x) | 1.0977 |
| C(6)-N | 1.4821 |
| C(6)-C(5) | 1.5526 |
| N-O(2) | 1.2410 |
| N-O(3) | 1.2418 |
| C(5)-H(5x) | 1.0969 |
| C(5)-H(5n) | 1.0945 |
| C(7)-H(7a) | 1.0960 |
| C(7)-H(7s) | 1.0960 |

TABLE 25. Selected angles (degrees) between bonded atoms of 6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (72).

| | |
|---|---|
| C(1)-C(6)-C(5) | 103.72 |
| C(5)-C(6)-H(6x) | 109.92 |
| C(1)-C(6)-H(6x) | 110.38 |
| C(1)-C(6)-N | 112.12 |
| C(5)-C(6)-N | 113.13 |
| O(2)-N-O(3) | 118.52 |
| H(6x)-C(6)-N | 107.58 |
| C(2)-O(1)-H | 121.50 |
| C(1)-C(2)-O(1) | 113.62 |
| C(3)-C(2)-O(1) | 111.49 |
| C(1)-C(7)-C(4) | 93.45 |
| C(1)-C(2)-C(3) | 102.79 |
| H(2x)-C(2)-O(1) | 107.42 |
| H(1)-C(1)-C(7) | 116.15 |
| C(3)-C(2)-H(2x) | 111.21 |
| C(1)-C(2)-H(2x) | 110.36 |

TABLE 26. Selected dihedral angles (degrees) for 6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (72).

| | |
|---|---|
| C(5)-C(6)-N-O(3) | 14.00 |
| H(6x)-C(6)-N-O(3) | 135.50 |
| C(3)-C(2)-O(1)-H | -174.10 |
| H(2x)-C(2)-O(1)-H | 63.80 |
| H(6x)-C(6)-C(5)-H(5x) | 10.30 |
| N-C(6)-C(1)-C(2) | 54.00 |
| O(1)-C(2)-C(1)-C(6) | -57.70 |
| C(1)-C(2)-C(3)-C(4) | 8.20 |
| C(1)-C(6)-C(5)-C(4) | -0.70 |
| H(1)-C(1)-C(7)-H(7s) | -60.60 |
| H(4)-C(4)-C(7)-H(7s) | 61.90 |

TABLE 27. Selected non-bonded distances (angstrom) for 6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (72).

| | |
|---|---|
| O(1)...O(2) | 3.1002 |
| O(1)...O(3) | 2.8014 |
| O(1)...N | 2.7150 |
| H...O(2) | 2.8470 |
| H...O(3) | 3.1210 |
| H...N | 2.8640 |

TABLE 28. Orthogonalised atomic coordinates for 3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (74).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.314529 | 2.576712 | 5.367439 |
| 3 | C(6) | 0.867062 | 0.794658 | 6.074071 |
| 4 | H(6x) | 0.308717 | 0.174267 | 5.355454 |
| 5 | H(6n) | 0.467467 | 0.474157 | 7.043225 |
| 6 | C(5) | 2.406508 | 0.609954 | 5.941284 |
| 7 | H(5n) | 2.910337 | 0.260304 | 6.857556 |
| 8 | H(5x) | 2.645387 | -0.161825 | 5.195631 |
| 9 | C(4) | 2.904607 | 2.003293 | 5.468240 |
| 10 | H(4) | 3.892153 | 1.984114 | 4.992680 |
| 11 | C(3) | 2.819327 | 3.022757 | 6.635849 |
| 12 | H(3x) | 3.216315 | 4.001016 | 6.336793 |
| 13 | N(1) | 3.587127 | 2.550525 | 7.818490 |
| 14 | O(1) | 4.762684 | 2.183517 | 7.646326 |
| 15 | O(2) | 3.263883 | 2.945993 | 8.953577 |
| 16 | C(2) | 1.288019 | 3.061417 | 6.903237 |
| 17 | C(8) | 0.783537 | 4.457093 | 6.999515 |
| 18 | H(1) | 0.999264 | 2.636071 | 7.870919 |
| 19 | C(7) | 1.734519 | 2.479964 | 4.567181 |
| 20 | H(7s) | 1.818812 | 3.513252 | 4.230589 |
| 21 | H(7a) | 1.514533 | 1.877618 | 3.695387 |
| 22 | N(2) | 0.357682 | 5.581267 | 7.181318 |

TABLE 29. Bond lengths (angstrom) for 3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (74).

| | |
|---|---|
| C(1)-H(1) | 1.0935 |
| C(1)-C(6) | 1.5484 |
| C(1)-C(2) | 1.5517 |
| C(1)-C(7) | 1.5426 |
| C(6)-H(6x) | 1.1014 |
| C(6)-H(6n) | 1.0963 |
| C(6)-C(5) | 1.5562 |
| C(5)-H(5x) | 1.0994 |
| C(5)-H(5n) | 1.1026 |
| C(5)-C(4) | 1.5535 |
| C(4)-H(4) | 1.0963 |
| C(4)-C(3) | 1.5517 |
| C(4)-C(7) | 1.5403 |
| C(3)-H(3x) | 1.0982 |
| C(3)-N(1) | 1.4867 |
| C(3)-C(2) | 1.5550 |
| N(1)-O(1) | 1.2447 |
| N(1)-O(2) | 1.2435 |
| C(2)-C(8) | 1.4872 |
| C(2)-H(2n) | 1.0958 |
| C(8)-N(2) | 1.2158 |
| C(7)-H(7s) | 1.0963 |
| C(7)-H(7a) | 1.0984 |

TABLE 30. Selected angles (degrees) between bonded atoms of 3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (74).

| | |
|---|---|
| C(4)-C(3)-N(1) | 111.23 |
| C(2)-C(3)-N(1) | 112.33 |
| C(2)-C(3)-C(4) | 101.55 |
| C(2)-C(3)-H(3x) | 112.34 |
| C(4)-C(3)-H(3x) | 111.13 |
| O(1)-N(1)-O(2) | 117.75 |
| C(1)-C(7)-C(4) | 93.70 |
| H(1)-C(1)-C(7) | 111.59 |
| H(3x)-C(3)-N(1) | 108.21 |
| C(3)-N(1)-O(2) | 118.14 |

TABLE 31. Selected dihedral angles (degrees) for 6-endo-nitro bicyclo[2.2.1]heptane-2-exo-carbonitrile, (74).

| | |
|---|---|
| C(2)-C(3)-N(1)-O(1) | -41.10 |
| O(1)-N(1)-C(3)-H(3x) | 83.30 |
| H(3x)-C(3)-C(2)-C(8) | -13.20 |
| N(1)-C(3)-C(4)-C(5) | 56.40 |
| H(5n)-C(5)-C(4)-C(3) | -52.60 |
| C(1)-C(2)-C(3)-C(4) | -10.30 |
| C(1)-C(6)-C(7)-H(7a) | -60.30 |
| H(4)-C(4)-C(7)-H(7a) | 61.80 |

TABLE 32. Orthogonalised coordinares for 3-exo-chloro-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (75).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.312529 | 2.576712 | 5.367439 |
| 3 | C(6) | 0.811030 | 0.791143 | 6.074071 |
| 4 | H(6x) | 0.129673 | 0.176912 | 5.465343 |
| 5 | H(6n) | 0.522585 | 0.584997 | 7.103352 |
| 6 | C(5) | 2.311025 | 0.496684 | 5.798494 |
| 7 | H(5n) | 2.873353 | 0.099478 | 6.655106 |
| 8 | H(5x) | 2.396748 | -0.286170 | 5.037811 |
| 9 | C(4) | 2.858449 | 1.845951 | 5.258298 |
| 10 | H(4) | 3.787287 | 1.722990 | 4.691828 |
| 11 | C(3) | 2.956803 | 2.874283 | 6.416169 |
| 12 | Cl | 3.736073 | 4.383566 | 5.849153 |
| 13 | N(1) | 3.750476 | 2.334832 | 7.554333 |
| 14 | O(1) | 4.858758 | 1.823551 | 7.312705 |
| 15 | O(2) | 3.559840 | 2.792253 | 8.711652 |
| 16 | C(2) | 1.453524 | 3.093472 | 6.782821 |
| 17 | C(8) | 1.099703 | 4.544597 | 6.813108 |
| 18 | H(2n) | 1.246588 | 2.727860 | 7.799159 |
| 19 | C(7) | 1.632703 | 2.366665 | 4.482680 |
| 20 | H(7s) | 1.718045 | 3.369363 | 4.042388 |
| 21 | H(7a) | 1.340021 | 1.717305 | 3.638102 |
| 22 | N(2) | 0.892975 | 5.741568 | 6.917927 |

TABLE 33. Bond lengths (angstrom) for 3-exo-chloro-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (75).

| | |
|---|---|
| C(1)-H(1) | 1.0917 |
| C(1)-C(6) | 1.5462 |
| C(1)-C(2) | 1.5526 |
| C(1)-C(7) | 1.5457 |
| C(6)-H(6x) | 1.1009 |
| C(6)-H(6n) | 1.0886 |
| C(6)-C(5) | 1.5533 |
| C(5)-H(5x) | 1.0949 |
| C(5)-H(5n) | 1.0990 |
| C(5)-C(4) | 1.5531 |
| C(4)-H(4) | 1.0949 |
| C(4)-C(3) | 1.5517 |
| C(4)-C(7) | 1.5412 |
| C(3)-Cl | 1.7909 |
| C(3)-N(1) | 1.4887 |
| C(3)-C(2) | 1.5628 |
| N(1)-O(2) | 1.2442 |
| N(1)-O(3) | 1.2590 |
| C(2)-C(8) | 1.4939 |
| C(2)-H(2n) | 1.0997 |
| C(8)-N(2) | 1.2192 |
| C(7)-H(7a) | 1.1048 |
| C(7)-H(7a) | 1.0984 |

TABLE 34. Selected angles (degrees) between bonded atoms for 3-exo-chloro-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (75).

| | |
|---|---|
| C(4)-C(3)-N(1) | 111.35 |
| C(2)-C(3)-N(1) | 112.60 |
| C(2)-C(3)-C(4) | 101.95 |
| C(2)-C(3)-Cl | 112.00 |
| C(4)-C(3)-Cl | 110.48 |
| O(1)-N(1)-O(2) | 117.56 |
| C(1)-C(7)-C(4) | 94.19 |
| h(1)-C(1)-C(7) | 107.77 |
| Cl-C(3)-N(1) | 108.39 |
| C(3)-N(1)-O(2) | 118.38 |

TABLE 35. Selected dihedral angles (degrees) for 3-exo-chloro-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (75).

| | |
|---|---|
| C(2)-C(3)-N(1)-O(1) | -41.70 |
| C(1)-C(3)-N(1)-O(1) | 82.80 |
| Cl-C(3)-C(2)-C(8) | -10.50 |
| N(1)-C(3)-C(4)-C(5) | 53.90 |
| H(5n)-C(5)-C(4)-C(3) | -53.50 |
| C(1)-C(2)-C(3)-C(4) | -5.70 |
| C(1)-C(6)-C(5)-C(4) | -1.70 |
| H(1)-C(1)-C(7)-H(7a) | -59.20 |
| H(4)-C(4)-C(7)-H(7a) | 59.40 |

TABLE 36. Orthogonalised atomic coordinates for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(4) | -0.318605 | 2.576712 | 5.367439 |
| 3 | C(3) | 0.833168 | 0.787925 | 6.074071 |
| 4 | Cl | -0.009679 | -0.237533 | 4.878701 |
| 5 | H(3n) | 0.407099 | 0.563628 | 7.057296 |
| 6 | C(2) | 2.373625 | 0.596058 | 5.994376 |
| 7 | O(1) | 2.905081 | 0.015573 | 7.193371 |
| 8 | H(2x) | 2.695145 | -0.076372 | 5.189144 |
| 9 | C(1) | 2.916858 | 2.016954 | 5.674271 |
| 10 | H(1) | 3.943959 | 2.012919 | 5.289813 |
| 11 | C(6) | 2.714801 | 3.059178 | 6.806461 |
| 12 | H(6x) | 3.144295 | 4.026762 | 6.515358 |
| 13 | N | 3.354685 | 2.646842 | 8.075706 |
| 14 | O(2) | 4.539698 | 2.278383 | 8.038007 |
| 15 | O(3) | 2.948550 | 3.144623 | 9.137893 |
| 16 | C(5) | 1.168511 | 3.128016 | 6.911456 |
| 17 | H(5x) | 0.819274 | 4.165581 | 6.847652 |
| 18 | H(5n) | 0.753440 | 2.796026 | 7.868684 |
| 19 | C(7) | 1.831111 | 2.499839 | 4.688522 |
| 20 | H(7a) | 1.941056 | 3.535789 | 4.347674 |
| 21 | H(7s) | 1.757698 | 1.916459 | 3.764095 |
| 22 | H | 2.625259 | 0.264196 | 8.058054 |

TABLE 37. Bond lengths (angstrom) between bonded atoms for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| C(4)-H(4) | 1.0972 |
| C(4)-C(3) | 1.5513 |
| C(4)-C(5) | 1.5510 |
| C(4)-C(7) | 1.5441 |
| C(3)-Cl | 1.7863 |
| C(3)-H(3n) | 1.0948 |
| C(3)-C(2) | 1.5544 |
| C(2)-O(1) | 1.4342 |
| C(2)-H(2x) | 1.0972 |
| C(2)-C(1) | 1.5545 |
| O(1)-H | 0.9422 |
| C(1)-H(1) | 1.0967 |
| C(1)-C(6) | 1.5521 |
| C(1)-C(7) | 1.5439 |
| C(6)-H(6x) | 1.0979 |
| C(6)-N | 1.4800 |
| C(6)-C(5) | 1.5514 |
| N-O(2) | 1.2415 |
| N-O(3) | 1.2414 |
| C(5)-H(5x) | 1.0966 |
| C(5)-H(5n) | 1.0949 |
| C(7)-H(7a) | 1.0961 |
| C(7)-H(7s) | 1.0956 |

TABLE 38. Selected angles (degrees) between bonded atoms of 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| C(1)-C(6)-N | 112.47 |
| C(5)-C(6)-N | 112.66 |
| C(2)-O(1)-H | 123.39 |
| C(1)-C(2)-O(1) | 114.37 |
| C(3)-C(2)-O(1) | 111.98 |
| C(5)-C(6)-C(1) | 102.06 |
| C(5)-C(6)-H(6x) | 111.64 |
| C(1)-C(6)-H(6x) | 110.33 |
| C(1)-C(2)-C(3) | 104.13 |
| C(1)-C(2)-H(2x) | 107.86 |
| C(3)-C(2)-H(2x) | 113.81 |
| O(3)-N-O(2) | 117.21 |
| C(6)-N-O(2) | 117.98 |
| C(1)-C(7)-C(4) | 93.42 |
| H(2x)-C(2)-O(1) | 104.89 |
| C(2)-C(1)-C(6) | 114.71 |
| C(5)-C(4)-C(3) | 107.88 |
| H(1)-C(1)-C(7) | 116.28 |

TABLE 39. Selected dihedral angles (degrees) for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| C(5)-C(6)-N-O(3) | -43.50 |
| H(6x)-C(6)-N-O(3) | 80.00 |
| C(3)-C(2)-O(1)-H | -41.50 |
| H(2x)-C(2)-O(1)-H | -165.40 |
| H(6x)-C(6)-C(5)-H(5x) | -10.00 |
| C(1)-C(2)-C(3)-C(4) | -8.00 |
| C(1)-C(6)-C(5)-C(4) | 3.30 |
| N-C(6)-C(1)-C(2) | 58.40 |
| O(1)-C(2)-C(1)-C(6) | -56.00 |
| H(1)-C(1)-C(7)-H(7s) | -61.90 |
| H(4)-C(4)-C(7)-H(7s) | 58.00 |

TABLE 40. Selected non-bonded distances (angstrom) for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| O(1)...O(2) | 2.9165 |
| O(1)...O(3) | 3.6843 |
| O(1)...N | 2.8110 |
| H...N | 2.4919 |
| H...O(2) | 2.7790 |
| H...O(3) | 3.0930 |

TABLE 38. Selected angles (degrees) between bonded atoms of 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| C(1)-C(6)-N | 112.47 |
| C(5)-C(6)-N | 112.66 |
| C(2)-O(1)-H | 123.39 |
| C(1)-C(2)-O(1) | 114.37 |
| C(3)-C(2)-O(1) | 111.98 |
| C(5)-C(6)-C(1) | 102.06 |
| C(5)-C(6)-H(6x) | 111.64 |
| C(1)-C(6)-H(6x) | 110.33 |
| C(1)-C(2)-C(3) | 104.13 |
| C(1)-C(2)-H(2x) | 107.86 |
| C(3)-C(2)-H(2x) | 113.81 |
| O(3)-N-O(2) | 117.21 |
| C(6)-N-O(2) | 117.98 |
| C(1)-C(7)-C(4) | 93.42 |
| H(2x)-C(2)-O(1) | 104.89 |
| C(2)-C(1)-C(6) | 114.71 |
| C(5)-C(4)-C(3) | 107.88 |
| H(1)-C(1)-C(7) | 116.28 |

TABLE 39. Selected dihedral angles (degrees) for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| C(5)-C(6)-N-O(3) | -43.50 |
| H(6x)-C(6)-N-O(3) | 80.00 |
| C(3)-C(2)-O(1)-H | -41.50 |
| H(2x)-C(2)-O(1)-H | -165.40 |
| H(6x)-C(6)-C(5)-H(5x) | -10.00 |
| C(1)-C(2)-C(3)-C(4) | -8.00 |
| C(1)-C(6)-C(5)-C(4) | 3.30 |
| N-C(6)-C(1)-C(2) | 58.40 |
| O(1)-C(2)-C(1)-C(6) | -56.00 |
| H(1)-C(1)-C(7)-H(7s) | -61.90 |
| H(4)-C(4)-C(7)-H(7s) | 58.00 |

TABLE 40. Selected non-bonded distances (angstrom) for 3-exo-chloro-6-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (77).

| | |
|---|---|
| O(1)...O(2) | 2.9165 |
| O(1)...O(3) | 3.6843 |
| O(1)...N | 2.8110 |
| H...N | 2.4919 |
| H...O(2) | 2.7790 |
| H...O(3) | 3.0930 |

TABLE 41. Orthogonalised atomic coordinates for 3-exo,6-exo-dichloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (7).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.311345 | 2.576712 | 5.367439 |
| 3 | C(6) | 0.882409 | 0.787445 | 6.074071 |
| 4 | Cl(1) | 0.391142 | -0.171987 | 4.617401 |
| 5 | H(6n) | 0.416753 | 0.289556 | 6.965144 |
| 6 | C(5) | 2.431417 | 0.696195 | 6.218029 |
| 7 | O(1) | 2.806308 | 0.045299 | 7.439700 |
| 8 | H(5x) | 2.931309 | 0.109332 | 5.428365 |
| 9 | C(4) | 2.898288 | 2.173754 | 6.138317 |
| 10 | H(4) | 3.995742 | 2.206507 | 6.041897 |
| 11 | C(3) | 2.375643 | 3.063215 | 7.327241 |
| 12 | Cl(2) | 3.101300 | 4.670961 | 7.262881 |
| 13 | N(1) | 2.719230 | 2.449706 | 8.650445 |
| 14 | O(2) | 3.919613 | 2.303353 | 8.945660 |
| 15 | O(3) | 1.866055 | 1.912138 | 9.386735 |
| 16 | C(2) | 0.841039 | 3.065500 | 7.046939 |
| 17 | C(8) | 0.394051 | 4.471266 | 6.850093 |
| 18 | H(2n) | 0.188928 | 2.618851 | 7.820401 |
| 19 | C(7) | 1.999409 | 2.665160 | 4.972716 |
| 20 | H(7s) | 2.084504 | 3.728355 | 4.723014 |
| 21 | H(7a) | 2.161311 | 2.158810 | 4.012840 |
| 22 | N(2) | 0.084265 | 5.631430 | 6.663974 |
| 23 | H | 3.703088 | 0.069567 | 7.746788 |

TABLE 42. Bond lengths (angstrom) for 3-exo,6-exo-dichloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (7).

| | |
|---|---|
| C(1)-H(1) | 1.0906 |
| C(1)-C(6) | 1.5572 |
| C(1)-C(2) | 1.5625 |
| C(1)-C(7) | 1.5495 |
| C(6)-Cl(1) | 1.8121 |
| C(6)-H(6n) | 1.1219 |
| C(6)-C(5) | 1.5584 |
| C(5)-O(1) | 1.4341 |
| C(5)-H(5x) | 1.1036 |
| C(5)-C(4) | 1.5516 |
| O(1)-H | 0.9482 |
| C(4)-H(4) | 1.1022 |
| C(4)-C(3) | 1.5574 |
| C(4)-C(7) | 1.5518 |
| C(3)-Cl(2) | 1.7925 |
| C(3)-N(1) | 1.4864 |
| C(3)-C(2) | 1.5603 |
| N(1)-O(2) | 1.2448 |
| N(1)-O(3) | 1.2486 |
| C(2)-C(8) | 1.4882 |
| C(2)-H(2n) | 1.1059 |
| C(8)-N(2) | 1.2151 |
| C(7)-H(7a) | 1.0973 |
| C(7)-H(7s) | 1.0954 |

TABLE 43. Selected angles (degrees) between bonded atoms of 3-exo,6-exo-dichloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (7).

| | |
|---|---|
| C(4)-C(3)-N(1) | 112.67 |
| C(2)-C(3)-N(1) | 113.29 |
| C(5)-O(1)-H | 120.76 |
| C(4)-C(5)-O(1) | 113.41 |
| C(6)-C(5)-O(1) | 111.41 |
| C(2)-C(3)-C(4) | 101.79 |
| C(2)-C(3)-Cl(2) | 111.89 |
| C(4)-C(3)-Cl(2) | 109.94 |
| C(4)-C(5)-C(6) | 103.80 |
| C(4)-C(5)-H(5x) | 109.47 |
| C(6)-C(5)-H(5x) | 114.54 |
| O(2)-N(1)-O(3) | 117.93 |
| C(3)-N(1)-O(2) | 118.69 |
| C(2)-C(1)-C(6) | 105.15 |
| C(3)-C(4)-C(5) | 112.66 |
| C(1)-C(7)-C(4) | 93.47 |
| H(1)-C(1)-C(7) | 124.45 |
| H(4)-C(4)-C(7) | 120.11 |

TABLE 44. Selected dihedral angles (degrees) for 3-exo,6-exo-dichloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (7).

| | |
|---|---|
| C(2)-C(3)-N(1)-O(3) | 7.30 |
| Cl(2)-C(3)-N(1)-O(3) | 131.30 |
| C(6)-C(5)-O(1)-H | -167.80 |
| H(5x)-C(5)-O(1)-H | 68.10 |
| N(1)-C(3)-C(4)-C(5) | 53.40 |
| O(1)-C(5)-C(4)-C(3) | -56.90 |
| Cl(2)-C(3)-C(2)-C(8) | -2.30 |
| C(1)-C(2)-C(3)-C(4) | -4.10 |
| C(1)-C(6)-C(5)-C(4) | 8.70 |
| H(1)-C(1)-C(7)-H(7a) | -70.40 |
| H(4)-C(4)-C(7)-H(7a) | 57.30 |

TABLE 45. Selected non-bonded distances (angstrom) for 3-exo,6-exo-dichloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (7).

| | |
|---|---|
| O(1)...O(2) | 2.9336 |
| O(1)...O(3) | 2.8566 |
| O(1)...N(1) | 2.6934 |
| H...N(1) | 2.7294 |
| H...O(2) | 2.5444 |
| H...O(3) | 3.0756 |

TABLE 46. Orthogonalised atomic coordinates for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.318941 | 2.576712 | 5.367439 |
| 3 | C(6) | 0.667356 | 0.785724 | 6.074071 |
| 4 | H(6x) | -0.067831 | 0.206065 | 5.494967 |
| 5 | H(6n) | 0.333435 | 0.655753 | 7.112506 |
| 6 | C(5) | 2.133905 | 0.357223 | 5.813316 |
| 7 | O(1) | 2.734787 | -0.220168 | 6.981387 |
| 8 | H(5x) | 2.126575 | -0.448159 | 5.059967 |
| 9 | C(4) | 2.817505 | 1.655681 | 5.288008 |
| 10 | H(4) | 3.731560 | 1.426861 | 4.720416 |
| 11 | C(3) | 2.988476 | 2.776631 | 6.361676 |
| 12 | Cl | 3.818074 | 4.198556 | 5.568200 |
| 13 | N(1) | 3.788462 | 2.321679 | 7.523608 |
| 14 | O(2) | 4.868455 | 1.744994 | 7.303435 |
| 15 | O(3) | 3.665255 | 2.911428 | 8.611733 |
| 16 | C(2) | 1.506174 | 3.097102 | 6.742405 |
| 17 | C(8) | 1.171425 | 4.536641 | 6.586884 |
| 18 | H(2n) | 1.237674 | 2.850985 | 7.777589 |
| 19 | C(7) | 1.633898 | 2.233396 | 4.479533 |
| 20 | H(7s) | 1.782520 | 3.195445 | 3.976208 |
| 21 | H(7a) | 1.288958 | 1.578461 | 3.666907 |
| 22 | N(2) | 0.917347 | 5.720720 | 6.497066 |
| 23 | H | 2.670967 | 0.170485 | 7.840898 |

TABLE 47. Bond lengths (angstrom) for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| C(1)-H(1) | 1.0975 |
| C(1)-C(6) | 1.5455 |
| C(1)-C(2) | 1.5538 |
| C(1)-C(7) | 1.5478 |
| C(6)-H(6x) | 1.1014 |
| C(6)-H(6n) | 1.0986 |
| C(6)-C(5) | 1.5502 |
| C(5)-O(1) | 1.4349 |
| C(5)-H(5x) | 1.1028 |
| C(5)-C(4) | 1.5586 |
| O(1)-H | 0.9463 |
| C(4)-H(4) | 1.1000 |
| C(4)-C(3) | 1.5616 |
| C(4)-C(7) | 1.5454 |
| C(3)-Cl | 1.7902 |
| C(3)-N(1) | 1.4822 |
| C(3)-C(2) | 1.5636 |
| N(1)-O(2) | 1.2440 |
| N(1)-O(3) | 1.2438 |
| C(2)-C(8) | 1.4861 |
| C(2)-H(2n) | 1.0974 |
| C(8)-N(2) | 1.2144 |
| C(7)-H(7a) | 1.0992 |
| C(7)-H(7s) | 1.0959 |

TABLE 48. Selected angles (degrees) between bonded atoms of 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| C(4)-C(3)-N(1) | 112.19 |
| C(2)-C(3)-N(1) | 112.56 |
| C(5)-O(1)-H | 123.03 |
| C(4)-C(5)-O(1) | 115.21 |
| C(6)-C(5)-O(1) | 111.76 |
| C(2)-C(3)-C(4) | 102.17 |
| C(2)-C(3)-Cl | 111.85 |
| C(4)-C(3)-Cl | 110.53 |
| C(4)-C(5)-C(6) | 103.93 |
| C(4)-C(5)-H(5x) | 112.40 |
| C(6)-C(5)-H(5x) | 108.12 |
| O(2)-N(1)-O(3) | 117.43 |
| C(3)-N(1)-O(2) | 118.17 |
| C(1)-C(7)-C(4) | 93.96 |
| H(1)-C(1)-C(4) | 109.24 |
| H(5x)-C(5)-O(1) | 105.37 |

TABLE 49. Selected dihedral angles (degrees) for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| C(2)-C(3)-N(1)-O(3) | -42.90 |
| C(6)-C(5)-O(1)-H | -46.80 |
| Cl-C(3)-N(1)-O(3) | 80.80 |
| H(5x)-C(5)-O(1)-H | -164.00 |
| Cl-C(3)-C(2)-C(8) | -6.80 |
| N(1)-C(3)-C(4)-C(5) | 58.50 |
| O(1)-C(5)-C(4)-C(3) | -53.20 |
| C(1)-C(2)-C(3)-C(4) | -3.20 |
| C(1)-C(6)-C(5)-C(4) | -1.30 |
| H(1)-C(1)-C(7)-H(7a) | -55.30 |
| H(4)-C(4)-C(7)-H(7a) | 58.80 |

TABLE 50. Selected non-bonded distances (angstrom) for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| O(1)...O(2) | 2.9186 |
| O(1)...O(3) | 3.6511 |
| O(1)...N(1) | 2.8045 |
| H...O(2) | 2.7562 |
| H...O(3) | 3.0159 |
| H...N(1) | 2.4448 |

TABLE 48. Selected angles (degrees) between bonded atoms of 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| C(4)-C(3)-N(1) | 112.19 |
| C(2)-C(3)-N(1) | 112.56 |
| C(5)-O(1)-H | 123.03 |
| C(4)-C(5)-O(1) | 115.21 |
| C(6)-C(5)-O(1) | 111.76 |
| C(2)-C(3)-C(4) | 102.17 |
| C(2)-C(3)-Cl | 111.85 |
| C(4)-C(3)-Cl | 110.53 |
| C(4)-C(5)-C(6) | 103.93 |
| C(4)-C(5)-H(5x) | 112.40 |
| C(6)-C(5)-H(5x) | 108.12 |
| O(2)-N(1)-O(3) | 117.43 |
| C(3)-N(1)-O(2) | 118.17 |
| C(1)-C(7)-C(4) | 93.96 |
| H(1)-C(1)-C(4) | 109.24 |
| H(5x)-C(5)-O(1) | 105.37 |

TABLE 49. Selected dihedral angles (degrees) for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| C(2)-C(3)-N(1)-O(3) | -42.90 |
| C(6)-C(5)-O(1)-H | -46.80 |
| Cl-C(3)-N(1)-O(3) | 80.80 |
| H(5x)-C(5)-O(1)-H | -164.00 |
| Cl-C(3)-C(2)-C(8) | -6.80 |
| N(1)-C(3)-C(4)-C(5) | 58.50 |
| O(1)-C(5)-C(4)-C(3) | -53.20 |
| C(1)-C(2)-C(3)-C(4) | -8.20 |
| C(1)-C(6)-C(5)-C(4) | -1.30 |
| H(1)-C(1)-C(7)-H(7a) | -55.30 |
| H(4)-C(4)-C(7)-H(7a) | 58.80 |

TABLE 50. Selected non-bonded distances (angstrom) for 3-exo-chloro-5-endo-hydroxy-3-endo-nitrobicyclo[2.2.1]heptane-2-exo-carbonitrile, (76).

| | |
|---|---|
| O(1)...O(2) | 2.9186 |
| O(1)...O(3) | 3.6511 |
| O(1)...N(1) | 2.8045 |
| H...O(2) | 2.7562 |
| H...O(3) | 3.0159 |
| H...N(1) | 2.4448 |

TABLE 51. Orthogonalised atomic coordinates for 5-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (82).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.317841 | 2.576712 | 5.367439 |
| 3 | C(2) | 0.787481 | 0.787037 | 6.074071 |
| 4 | H(2x) | 0.291764 | 0.154820 | 5.325465 |
| 5 | O(1) | 0.203518 | 0.509959 | 7.354345 |
| 6 | C(3) | 2.317093 | 0.553739 | 6.102083 |
| 7 | H(3n) | 2.688684 | 0.197304 | 7.067618 |
| 8 | H(3x) | 2.609172 | -0.248909 | 5.414164 |
| 9 | C(4) | 2.896372 | 1.916462 | 5.643680 |
| 10 | H(4) | 3.914849 | 1.845413 | 5.243474 |
| 11 | C(5) | 2.766387 | 2.963804 | 6.779175 |
| 12 | H(5x) | 3.283887 | 3.895211 | 6.516184 |
| 13 | N | 3.334379 | 2.459068 | 8.051134 |
| 14 | O(2) | 4.459583 | 1.934893 | 8.025989 |
| 15 | O(3) | 2.981304 | 2.993678 | 9.114430 |
| 16 | C(6) | 1.228638 | 3.154685 | 6.864517 |
| 17 | H(6x) | 0.954888 | 4.208461 | 6.733686 |
| 18 | H(6n) | 0.783867 | 2.903384 | 7.832395 |
| 19 | C(7) | 1.815391 | 2.408201 | 4.659416 |
| 20 | H(7a) | 1.969730 | 3.424080 | 4.278364 |
| 21 | H(7s) | 1.691002 | 1.776122 | 3.772812 |
| 22 | H | -0.706609 | 0.687039 | 7.530044 |

TABLE 52. Bond lengths (angstrom) for 5-endo-nitrobicyclo-[2.2.1]heptan-2-endo-ol, (82).

| | |
|---|---|
| C(1)-H(1) | 1.0965 |
| C(1)-C(2) | 1.5484 |
| C(1)-C(6) | 1.5497 |
| C(1)-C(7) | 1.5419 |
| C(2)-H(2x) | 1.0981 |
| C(2)-O(1) | 1.4342 |
| O(1)-H | 0.9437 |
| C(3)-H(3x) | 1.0967 |
| C(3)-H(3n) | 1.0943 |
| C(3)-C(4) | 1.5501 |
| C(4)-H(4) | 1.0966 |
| C(4)-C(5) | 1.5502 |
| C(4)-C(7) | 1.5424 |
| C(5)-H(5x) | 1.0975 |
| C(5)-N | 1.4816 |
| C(5)-C(6) | 1.5519 |
| N-O(2) | 1.2416 |
| N-O(3) | 1.2414 |
| C(6)-H(6x) | 1.0966 |
| C(6)-H(6n) | 1.0944 |
| C(7)-H(7a) | 1.0959 |
| C(7)-H(7s) | 1.0959 |

TABLE 53. Selected angles (degrees) between bonded atoms of 5-endo-nitrobicyclo[2.2.1]heptane-2-endo-ol, (82).

| | |
|---|---|
| C(4)-C(5)-N | 111.50 |
| C(6)-C(5)-N | 111.99 |
| C(2)-O(1)-H | 121.51 |
| C(3)-C(2)-O(1) | 110.93 |
| C(1)-C(2)-O(1) | 112.03 |
| C(4)-C(5)-C(6) | 101.92 |
| C(6)-C(5)-H(5x) | 112.09 |
| C(4)-C(5)-H(5x) | 110.99 |
| C(1)-C(7)-C(4) | 93.28 |
| C(2)-C(1)-C(6) | 109.81 |
| C(5)-C(4)-C(3) | 110.24 |
| H(1)-C(1)-C(7) | 116.34 |
| H(4)-C(4)-C(7) | 116.02 |

TABLE 54. Selected dihedral angles (degrees) for 5-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (82).

| | |
|---|---|
| C(6)-C(5)-N-O(3) | -161.30 |
| H(5x)-C(5)-N-O(3) | 77.80 |
| C(1)-C(2)-O(1)-H | 59.90 |
| H(2x)-C(2)-O(1)-H | -63.30 |
| H(5x)-C(5)-C(6)-H(6x) | -5.10 |
| N-C(5)-C(4)-C(3) | -52.00 |
| O(1)-C(2)-C(1)-C(6) | 51.20 |
| C(1)-C(2)-C(3)-C(4) | -3.90 |
| C(1)-C(6)-C(5)-C(4) | -4.40 |
| H(1)-C(1)-C(7)-H(7s) | -61.90 |
| H(4)-C(4)-C(7)-H(7s) | 60.10 |

TABLE 55. Selected non-bonded distances (angstrom) for 5-endo-nitrobicyclo[2.2.1]heptan-2-endo-ol, (82).

| | |
|---|---|
| O(1)...O(2) | 4.538 |
| O(1)...O(3) | 4.121 |

TABLE 56. Orthogonalised atomic coordinates for 2-exo-nitrobicyclo[2.2.1]heptan-7-syn-ol, (83).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(4) | 0.965617 | 4.138398 | 3.370607 |
| 2 | H(4) | 1.936030 | 4.586813 | 3.615082 |
| 3 | C(5) | 0.991479 | 3.267337 | 2.091350 |
| 4 | H(5x) | 1.595833 | 3.732485 | 1.303277 |
| 5 | H(5n) | 1.465673 | 2.291022 | 2.240366 |
| 6 | C(6) | -0.505620 | 3.191580 | 1.699604 |
| 7 | H(6n) | -0.886504 | 2.171982 | 1.574639 |
| 8 | H(6x) | -0.690922 | 3.651093 | 0.721015 |
| 9 | C(1) | -1.199411 | 3.992451 | 2.829423 |
| 10 | H(1) | -2.211872 | 4.312017 | 2.557886 |
| 11 | C(2) | -1.126162 | 3.143355 | 4.128156 |
| 12 | N | -1.993327 | 3.720739 | 5.185568 |
| 13 | H(2n) | -1.440247 | 2.105431 | 3.968216 |
| 14 | C(3) | 0.370828 | 3.283417 | 4.515957 |
| 15 | H(3x) | 0.509637 | 3.794735 | 5.475055 |
| 16 | H(3n) | 0.883020 | 2.326792 | 4.666575 |
| 17 | C(7) | -0.175525 | 5.124990 | 3.053997 |
| 18 | O(1) | -0.498291 | 5.955259 | 4.178717 |
| 19 | H | -1.319034 | 6.417739 | 4.226016 |
| 20 | H(7a) | 0.010601 | 5.763442 | 2.181675 |
| 21 | O(2) | -1.806580 | 3.371515 | 6.362233 |
| 22 | O(3) | -3.133133 | 4.110557 | 4.885786 |

TABLE 57. Bond lengths (angstrom) for 2-exo-nitrobicyclo[2.2.1]heptan-7-syn-ol, (83).

| | |
|---|---|
| C(4)-H(4) | 1.0966 |
| C(4)-C(5) | 1.5478 |
| C(4)-C(3) | 1.5480 |
| C(4)-C(7) | 1.5414 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(5)-C(6) | 1.5494 |
| C(6)-H(6x) | 1.0969 |
| C(6)-H(6n) | 1.0956 |
| C(6)-C(1) | 1.5489 |
| C(1)-H(1) | 1.0959 |
| C(1)-C(2) | 1.5534 |
| C(1)-C(7) | 1.5432 |
| C(2)-N | 1.4844 |
| C(2)-H(2n) | 1.0961 |
| C(2)-C(3) | 1.5527 |
| N-O(2) | 1.2415 |
| N-O(3) | 1.2414 |
| C(3)-H(3x) | 1.0957 |
| C(3)-H(3n) | 1.0955 |
| C(7)-O(1) | 1.4348 |
| C(7)-H(7a) | 1.0969 |
| O(1)-H | 0.9433 |

TABLE 58. Selected angles (degrees) between bonded atoms of 2-exo-nitrobicyclo[2.2.1]heptan-7-syn-ol, (83).

| | |
|---|---|
| O(2)-N-O(3) | 117.09 |
| H(2n)-C(2)-N | 107.75 |
| C(1)-C(2)-N | 110.82 |
| C(3)-C(2)-N | 110.49 |
| C(2)-N-O(3) | 119.11 |
| H(7a)-O(1)-H | 121.25 |
| C(1)-C(7)-C(4) | 92.94 |
| C(2)-C(1)-C(6) | 107.82 |
| C(3)-C(4)-C(5) | 107.89 |
| H(1)-C(1)-C(7) | 115.79 |
| H(4)-C(4)-C(7) | 116.05 |
| C(4)-C(7)-O(1) | 112.08 |
| H(7a)-C(7)-O(1) | 108.95 |

TABLE 59. Selected dihedral angles (degrees) for 2-exo-nitrobicyclo[2.2.1]heptan-7-syn-ol, (83).

| | |
|---|---|
| C(3)-C(2)-N-O(3) | 155.90 |
| C(3)-C(2)-N-O(2) | -50.50 |
| C(1)-C(2)-N-O(3) | 43.80 |
| C(1)-C(2)-N-O(2) | -162.60 |
| H(2n)-C(2)-N-O(3) | -79.70 |
| H(2n)-C(2)-N-O(2) | 74.00 |
| H(7a)-C(7)-O(1)-H | 70.80 |
| C(2)-C(1)-C(7)-O(1) | -61.50 |
| C(1)-C(2)-C(3)-C(4) | -2.20 |
| C(1)-C(6)-C(5)-C(4) | -1.70 |
| H(1)-C(1)-C(2)-N | -43.10 |
| H(3x)-C(3)-C(2)-N | -1.20 |
| H(4-)C(4)-C(7)-O(1) | -63.00 |

TABLE 60. Selected non-bonded distances (angstrom) for 2-exo-nitrobicyclo[2.2.1]heptan-7-syn-ol, (83).

| | |
|---|---|
| O(1)...O(2) | 3.6270 |
| O(1)...O(3) | 3.2930 |
| H...O(3) | 3.0080 |

TABLE 61. Orthogonalised atomic coordinates for bicyclo[2.2.1]-heptan-2-endo-ol, (70).

| | | x | y | z |
|---|---|---|---|---|
| 1 | C(1) | 0.685443 | 2.286513 | 5.701483 |
| 2 | H(1) | -0.317821 | 2.576712 | 5.367439 |
| 3 | C(2) | 0.791099 | 0.786278 | 6.074710 |
| 4 | H(2) | 0.281807 | 0.155106 | 5.333841 |
| 5 | O | 0.225649 | 0.513217 | 7.363450 |
| 6 | H | -0.681416 | 0.692391 | 7.552326 |
| 7 | C(3) | 2.319311 | 0.538686 | 6.078946 |
| 8 | H(3n) | 2.708470 | 0.184733 | 7.039363 |
| 9 | H(3x) | 2.601584 | -0.256251 | 5.378310 |
| 10 | C(4) | 2.895324 | 1.906036 | 5.636631 |
| 11 | H(4) | 3.916515 | 1.843083 | 5.241505 |
| 12 | C(5) | 2.753243 | 2.698548 | 6.815028 |
| 13 | H(5x) | 3.319090 | 3.818937 | 6.626770 |
| 14 | H(5n) | 3.172433 | 2.524040 | 7.755398 |
| 15 | C(6) | 1.227581 | 3.161162 | 6.859387 |
| 16 | H(6x) | 0.993839 | 4.220258 | 6.696206 |
| 17 | H(6n) | 0.766479 | 2.942649 | 7.828323 |
| 18 | C(7) | 1.815889 | 2.416141 | 4.660897 |
| 19 | H(7a) | 1.980852 | 3.435982 | 4.295294 |
| 20 | H(7s) | 1.686578 | 1.795565 | 3.766967 |

TABLE 62. Bond lengths (angstrom) for bicyclo[2.2.1]heptan-2-endo-ol, (70).

| | |
|---|---|
| C(1)-H(1) | 1.0965 |
| C(1)-C(2) | 1.5494 |
| C(1)-C(6) | 1.5491 |
| C(1)-C(7) | 1.5419 |
| C(2)-H(2x) | 1.0980 |
| C(2)-O | 1.4342 |
| O-H | 0.9437 |
| C(2)-C(3) | 1.5481 |
| C(3)-H(3x) | 1.0966 |
| C(3)-H(3n) | 1.0950 |
| C(3)-C(4) | 1.5483 |
| C(4)-H(4) | 1.0968 |
| C(4)-C(7) | 1.5419 |
| C(4)-C(5) | 1.5472 |
| C(5)-H(5x) | 1.0967 |
| C(5)-H(5n) | 1.0956 |
| C(5)-C(6) | 1.5487 |
| C(6)-H(6x) | 1.0968 |
| C(6)-H(6n) | 1.0951 |
| C(7)-H(7s) | 1.0954 |
| C(7)-H(7a) | 1.0959 |

TABLE 63. Selected angles (degrees) between bonded atoms of bicyclo[2.2.1]heptan-2-endo-ol, (70).

| | |
|---|---|
| C(2)-O-H | 121.5180 |
| C(3)-C(2)-O | 110.8497 |
| C(1)-C(2)-O | 111.9418 |
| C(4)-C(5)-C(6) | 102.7707 |
| C(6)-C(5)-H(5x) | 111.7699 |
| C(4)-C(5)-H(5x) | 111.1147 |
| C(1)-C(7)-C(4) | 93.3495 |
| C(2)-C(1)-C(6) | 110.0653 |
| C(5)-C(4)-C(3) | 108.3474 |
| H(1-)C(1)-C(7) | 116.2924 |
| H(4-)C(4)-C(7) | 116.2849 |

TABLE 64. selected dihedral angles (degrees) for bicyclo[2.2.1]heptan-2-endo-ol, (70).

| | |
|---|---|
| C(1)-C(2)-O-H | 59.89 |
| H(2x)-C(2)-O-H | -61.10 |
| H(5x)-C(5)-C(6)-H(6x) | -0.10 |
| O-C(2)-C(1)-C(6) | 50.50 |
| C(1)-C(2)-C(3)-C(4) | -2.90 |
| C(1)-C(5)-C(5)-C(4) | 0.00 |
| H(1-)C(1)-C(7)-H(7s) | -61.30 |
| C(3)-C(2)-O-H | 174.10 |

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