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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