SUPPLEMENTARY MATERIAL

Comment on "Penicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theory" by Z. Mucsi, G. A. Chass, P. Ábrányi-Balogh, B. Jójárt, D.-C. Fang, A. J. Ramirez-Cuesta, B. Viskolczc and I. G. Csizmadia, Phys. Chem. Chem. Phys., 2013, 15, 20447

Stephen A. Glover

Department of Chemistry, School of Science and Technology, University of New England, Armidale, New South Wales, 2350, Australia; Email: sglover@une.edu.au

Table of contents

Table S1 Strain enthalpies for hydrogenation reactions in Table 1 and Table 2 3

Table S2 B3LYP/6-31G(d,p) data for hydrogenation enthalpies in Table 1 and Eq. 7 4

Table S3. B3LYP/6-31G(d,p) enthalpies for TA and COSNAR data in Table 1 and for 6-acetamidopenicillanic acid 15 6

Table S4. B3LYP/6-31G(d,p) TA and COSNAR results for Table 1 and for 6-acetamidopenicillanic acid 15 using enthalpies in Table S3 8

Table S5 B3LYP/6-31G(d) energies (au) for TA and COSNAR data in Table 4 9

Table S6 B3LYP/6-31G(d) energies (au) for TA and COSNAR data for 30, 31 and 32a in Table 6 11

Table S7. B3LYP/6-31G(d) TA and COSNAR results for 30, 31 and 32a in Table 6 12

Table S8 B3LYP/6-31G(d,p) structures for strain enthalpies, ΔH^{RS} in Table 1 13

Table S9 B3LYP/6-31G(d,p) structures for hydrogenation enthalpies, ΔH^{obs} in Table 1 and Table 2 and Eq. 7 14

Table S10 B3LYP/6-31G(d,p) Enthalpy Structures for TA-COSNAR data in Table 1 16

Table S11 B3LYP/6-31G(d,p) conformers and structures for hydrogenation enthalpies, ΔH^{obs} in Table 2 22

Table S12. Energies for derivation of TA and COSNAR resonance energies of 3a and 6 in Table 3 25

Table S12 B3LYP/6-31G(d) structures for TA and COSNAR data in Table 4 and Table 6.....28

B3LYP/6-31G(d,p) vibrational frequencies.....48

Table S1 Strain enthalpies for hydrogenation reactions in Table 1 and Table 2

□ΔH^{RS}=2625x(B+D)-(A+C))

β-Propiolactam **3a**		E (au)	Hº (au)	
A	cyclobutanone	-231.237181	-231.14066	
B	Butanone	-232.481887	-232.362492	
C	2-Butanol	-233.685267	-233.541143	
D	Cyclobutanol	-232.439669	-232.318295	
	$\Delta E^{RS}/\Delta H^{RS}$	2.34191032	2.667467	kJ/mol
γ-Butyrolactam **4a**		E (au)	Hº (au)	
A	cyclopentanone	-270.584115	-270.456450	
D	Cyclopentanol	-271.784794	-271.632647	
	$\Delta E^{RS}/\Delta H^{RS}$	0.56972482	6.4455043	kJ/mol
δ-Valeroactam **5a**		E (au)	Hº (au)	
A	Cyclohexanone	-309.905312	-309.747328	
D	Cyclohexanol	-311.111238	-310.92874	
	$\Delta E^{RS}/\Delta H^{RS}$	-6.68442116	-7.24889506	$kJmol^{-1}$
N-Acetyl-β-propiolactam **3c**		E (au)	Hº (au)	
A	2-Acetylcyclobutanone	-383.884918	-383.748168	
D	2-Acetylcyclobutanol	-385.086881	-384.925561	
	$\Delta E^{RS}/\Delta H^{RS}$	-3.720276	-3.30282868	kJ/mol
6-Acetamidopenicillanic acid (from Eq. 9)		E (au)	Hº (au)	
A	7-acetamido-6-oxo-2-thia-bicyclo[3.2.0]heptane	-914.869152	-914.673874	
D	7-acetamido-6-hydroxy-2-thiabicyclo[3.2.0]heptane	-916.072097	-915.852724	
	$\Delta E^{RS}/\Delta H^{RS}$	1.1420751	-0.52246654	$kJmol^{-1}$

Table S2 B3LYP/6-31G(d,p) data for hydrogenation enthalpies in Table 1 and Eq. 7

ΔH^{obs}(kJmol^{-1}) = 2625 × (B-(A+C))

ΔH^{RE} (kJmol^{-1}) = ΔH^{obs}–ΔH^{RS}

Amidicity(%)=ΔH^{RE} × 1.258+56.126

RE (kJmol^{-1}) = –Amidicity/1.258

β-Propiolactam 3a		E (au)	Hº (au)
A	**3a**	-247.294715	-247.208561
B	**3a+H_2**	-248.469550	-248.359642
C	H_2	-1.178541	-1.165063
	ΔH^{obs} (kJmol^{-1})		36.702907
	ΔH^{RS} (kJmol^{-1})		2.667467
	ΔH^{RE} (kJmol^{-1})		34.035440
	Amidicity (%)		98.942583
	RE (kJmol^{-1})		-78.650702
***N*-Methyl-β-propiolactam 3b**		E (au)	Hº (au)
A	**3b**	-286.611140	-286.495566
B	**3b+H_2**	-287.783207	-287.644386
C	H_2	-1.178541	-1.165063
	ΔH^{obs} (kJmol^{-1})		42.638032
	ΔH^{RS} (kJmol^{-1})		2.667467
	ΔH^{RE} (kJmol^{-1})		39.970565
	Amidicity (%)		106.408970
	RE (kJmol^{-1})		-84.585827
γ-Butyrolactam 4a		E (au)	Hº (au)
A	**4a**	-286.641737	-286.524446
B	**4a+H_2**	-287.814170	-287.673786
C	Hydrogen	-1.178541	-1.165063
	ΔH^{obs} (kJmol^{-1})		41.273032
	ΔH^{RS} (kJmol^{-1})		6.445504
	ΔH^{RE} (kJmol^{-1})		34.827528
	Amidicity (%)		99.939030
	RE (kJmol^{-1})		-79.442790
δ-Valerolactam 5a		E(au)	Hº (au)
A	**5a**	-325.960564	-325.812988
B	**5a+H_2**	-327.138215	-326.967308
C	H_2	-1.178541	-1.165063
	ΔH^{obs} (kJmol^{-1})		28.200532

	ΔH^{RS} (kJmol^{-1})			-7.248895
	ΔH^{RE} (kJmol^{-1})			35.449427
	Amidicity (%)			100.721379
	RE (kJmol^{-1})			–80.064689
***N*-Acetyl-β-propiolactam 3c**		E (au)		Hº (au)
A	**3c**		-399.959426	-399.832956
B	**3c+H_2** (lactam)		-401.140955	-400.990884
C	H_2		-1.178541	-1.165061
	ΔH^{obs} (kJmol^{-1})		18.750011	18.725726
	ΔH^{RS} (kJmol^{-1})		-20.36	-3.302828
	ΔH^{RE} (kJmol^{-1})		-1.609988	22.028554
	Amidicity (%)			83.837922
	RE (kJmol^{-1})			66.643817
		E (au)		Hº (au)
B	**3c+H_2** (amide)		-401.144731	-400.994310
C	H_2		-1.178541	-1.165061
	ΔH^{obs}=ΔH^{RE} (kJmol^{-1})			9.732476
	Amidicity (%)			68.369455
	RE (kJmol^{-1})			54.347738
Dimethylacetamide 1		E (au)		Hº (au)
D	**1**		-287.842522	-287.704235
E	**1 + H_2**		-289.016946	-288.855209
	ΔH^{diff} (Eq. 7)			
	2625x[(B(**3a**)+D-(A(**3a**)+E)]			-0.280875

Table S3 B3LYP/6-31G(d,p) enthalpies for TA and COSNAR data in Table 1 and for 6-acetamidopenicillanic acid 15

Key	Structure	E(au)	H^o(au)
[1]	**β-Propiolactam 3a**		
A	Azetidine	-173.2492	-173.144349
B	β-Propiolactam	-247.294715	-247.208561
C	Cyclobutanone	-231.237181	-231.140660
D	Cyclobutane	-157.224581	-157.108573
E	Butane	-158.471951	-158.333185
F	Butanone	-233.684292	-232.362492
G	*N*,*N*-dimethylacetamide	-287.842522	-287.704235
H	*N*,*N*-dimethylethylamine	-213.803286	-213.646729
[2]	***N*-Methyl-β-Propiolactam 3b**		
A	*N*-Methylazetidine	-212.564323	-212.430725
B	*N*-Methyl-β-propiolactam	-286.61114	-286.495566
C	2-Methylcyclobutanone	-270.55665	-270.43037
D	Methylcyclobutane	-196.544347	-196.399222
[3]	**γ-Butyrolactam 4a**		
A	Pyrolidine	-212.596121	-212.46072
B	γ-Butyrolactam	-286.641737	-286.524446
C	Cyclopentanone	-270.584116	-270.456451
D	Cyclopentane	-196.57113	-196.424397
[4]	**δ-Valerolactam 5a**		
A	Piperidine	-251.921312	-251.755398
B	δ-Valerolactam	-325.960564	-325.812988
C	Cyclohexanone	-309.905312	-309.747328
D	Cyclohexane	-235.897276	-235.720187
[5]	***N*-Acetyl-β-propiolactam 4c *endo***		
A	*N*-Acetylazetidine	-325.921599	-325.77663
B	*N*-Acetyl-β-propiolactam	-399.959426	-399.832952
C	2-Acetylcyclobutanone	-383.884918	-383.748168
D	Acetylcyclobutane	-309.870619	-309.714736
[6]	***N*-Acetyl-β-propiolactam 4c *exo***		
A	*N*-Ethyl-β-propiolactam	-325.929975	-325.784789
D	2-Ethylcyclobutanone	-309.873425	-309.71753
[7]	***N*-Acetyl-β-propiolactam 4c *exo/endo*[c]**		
A	*N*-Ethylazetidine	-251.883334	-251.720284
D	Ethylcyclobutane	-235.860761	-235.685889
[8]Scheme	***N*-1-Hydroxyethyl-β-propiolactam**		

3(path i)			
A	*N*-(1-Hydroxyethyl)azetidine	-327.099	-326.930837
B	*N*-(1-Hydroxyethyl)-β-propiolactam	-401.144731	-400.99431
C	2-(1-Hydroxyethyl)cyclobutanone	-385.086686	-384.925597
D	1-Cyclobutylethanol	-311.074435	-310.894183
[9]Scheme 3(path ii)	***N*-Acetyl-2-hydroxyazetidine**		
A	2-Ethyl-2-hydroxyazetidine	-327.103999	-326.935738
B	*N*-Acetyl-2-hydroxyazetidine	-401.141368	-400.991347
C	2-Acetylcyclobutanol	-385.086903	-384.925583
D	2-Ethylcyclobutanol	-311.076235	-310.895879
[10]	**6-Acetamidopenicillanic acid 15**		
A	6-Acetamido-1-aza-3,3-dimethyl-4-thia bicyclo[3.2.0]heptane-2-carboxylic acid	-1123.8106	-1123.8106
B	6-Acetamidopenicillanic acid	-1197.8576	-1197.8576
C	7-Acetamido-3,3-dimethyl-2-thia bicyclo[3.2.0]heptan-6-one-4-carboxylic acid	-1181.80182	-1181.80182
D	7-Acetamido-3,3-dimethyl-2-thia bicyclo[3.2.0]heptane-4-carboxylic acid	-1107.77255	-1107.77255

Table S4. B3LYP/6-31G(d,p) TA and COSNAR results for Table 1 and for 6-acetamidopenicillanic acid 15 using enthalpies in Table S3

Dataset (Table S3)		[1]	[2]	[3]	[4]	[5]	[6]	[7][c]	[8]	[9]	[10]
		3a	**3b**	**4a**	**5a**	**3c$_{endo}$**	**3c$_{exo}$**	**3c**	Scheme 3(i)	Scheme 3(ii)	**15**
□□□H_{obs}/kJmol^{-1}	2625×((B+H)-(A+G))	-17.60	-19.25	-16.33	-0.22	3.11	24.53	6.14	-15.66	4.98	27.58
□□□H_{corr}/kJmol^{-1}	2625×(C+E)-(D+F))	-7.30	-4.83	-7.21	5.69	-10.83	0.00	-9.62	-5.53	0.00	0.10
□□□H_{TA}/kJmol^{-1}	□□H_{obs}–□H_{corr}	-10.31	-14.42	-9.12	-5.91	13.94	24.53	15.76	-10.13	4.98	27.49
RE_{TA}/kJmol^{-1}							–				
	–(77.47[a]–E_{TA})	–87.78	–91.90	–86.59	–83.38	–63.54	52.95	–139.19	–87.61	–72.49	–49.56
RE_{COSNAR}kJmol^{-1}							–				
	2625((B+D)–(A+C))	–84.34	–88.46	–83.15	–79.94	–60.10	46.01	–132.31	–84.17	–68.01	–46.55
Amidicity$_{TA}$/%	100x(RE_{TA}/–77.47[a])	113.30	118.62	111.77	107.62	82.01	68.34	179.66	113.08	93.57	60.08
Amidicity$_{COSNAR}$/%			-	-	-						
	100x(RE_{COSNAR}/–76.27[b])	-110.58	115.98	109.02	104.81	78.79	60.33	173.48	110.36	89.17	61.03

[a] TA enthalpy of 1-azaadamantan-2-one at B3LYP/6-31G(d,p)

[b] COSNAR enthalpy *N*,*N*-dimethylacetamide at B3LYP/6-31G(d,p)

[c] TA requires ΔE_{obs} = 2625×((B+2H)-(A+2G)); ΔE_{corr}=2625×(C+2E)-(D+2F)); RE_{TA}=–(2x77.47–E_{TA})

Table S5 B3LYP/6-31G(d) energies (au) for TA and COSNAR data in Table 4

ΔE_{obs}/kJmol^{-1} = 2625×((B+H)-(A+G))

ΔE_{corr}/kJmol^{-1} = 2625×(C+E)-(D+F))

ΔE_{TA}/kJmol^{-1} = E_{obs}–E_{corr}

RE_{TA}/kJmol^{-1}= –(76.03[a]a–ΔE_{TA})

RE_{COSNAR}kJmol^{-1} = 2625((B+D)-(A+C))

$Amidicity_{TA}$/% = 100x(RE_{TA}/–76.03

$Amidicity_{COSNAR}$/% = 100x(RE_{COSNAR}/–77.51[b])

			Axial	Equatorial
	Penam **6** ax		[1]	[2]
A	4-Thia-1-azabicyclo[3.2.0]heptane (Penamine)		-648.85282	-648.848705
B	7-Oxo-4-thia-1-azabicyclo[3.2.0]heptane (Penam)		-722.892151	-722.890072
C	5-Thiabicyclo[3.2.0]heptan- 2-one (Penone)		-706.839829	-706.836902
D	2-Thiabicyclo[3.2.0]heptane (Penane)		-632.82636	-632.824358
E	Butane	-158.4580463		
F	Butanone	-232.4705593		
G	*N*,*N*-dimethylacetamide	-213.788638		
H	*N*,*N*-dimethylethylamine	-287.830189		
	Penam-3-carboxylic acid **23** HB		[3]	[4]
A	Penamine		-837.41879	-837.41653
B	Penam		-911.451791	-911.449799
C	Penone		-895.397454	-895.400466
D	Penane		-821.386541	-821.389486
	Penam-3-carboxylic acid **24** NHB		[5]	[6]
A	Penamine		-837.414975	-837.413372
B	Penam		-911.453675	-911.4518
C	Penone		-895.404235	-895.400466
D	Penane		-821.390097	-821.389486
	2,2-Dimethylpenam **25**		[7]	[8]
A	Penamine		-727.478255	-727.477605
B	Penam		-801.521718	-801.519576
C	Penone		-785.467595	-785.466494
D	Penane		-711.45242	-711.453629
	Penicillanic acid **26** HB		[9]	[10]

A	Penamine	-916.039943	-916.046448
B	Penam	-990.075865	-990.079713
C	Penone	-974.028153	-974.021895
D	Penane	-900.01303	-900.008993
	Penicillanic acid **26** NHB	[11]	[12]
A	Penamine	-916.038729	-916.039648
B	Penam	-990.081673	-990.080223
C	Penone	-974.028153	-974.021895
D	Penane	-900.01303	-900.008993
	6-Acetamido-2,2-dimethylpenam **28**	[13]	[14]
A	Penamine	-935.494125	-935.492649
B	Penam	-1009.53367	-1009.53181
C	Penone	-993.481553	-993.48132
D	Penane	-919.469091	-919.468643
	6-Acetamido-2,2-dimethylpenam-3-carboxylic acid **15** HB	[15]	[16]
A	Penamine	-1124.05419	-1124.05997
B	Penam	-1198.08719	-1198.09125
C	Penone	-1182.03542	-1182.04514
D	Penane	-1108.02374	-1108.0321
	6-Acetamido-2,2-dimethylpenam-3-carboxylic acid **14** NHB	[17]	[18]
A	Penamine	-1124.05426	-1124.05384
B	Penam	-1198.09341	-1198.09186
C	Penone	-1182.04204	-1182.04514
D	Penane	-1108.02973	-1108.0321
	6-Acetamido-2,2-dimethylpenam-3-carboxylate **16**	[19]	
A	Penamine	-1123.49737	
B	Penam	-1197.54834	
C	Penone	-1181.49784	
D	Penane	-1107.47918	
	6-Acetamido-*N,N*,2,2-tetramethylpenam-3-carboxamide **29b**	[20]	

A	Penamine	-1182.80041
B	Penam	-1256.84155
C	Penone	-1240.78937
D	Penane	-1166.77579

Table S6 B3LYP/6-31G(d) energies (au) for TA and COSNAR data for 30, 31 and 32a in Table 6

	1-Azabicyclo[3.3.1]nonan-2-one **30** (Table 6)	[1]
A	1-Azabicyclo[3.3.1]nonane	-368.622795
B	1-Azabicyclo[3.3.1]nonan-2-one	-442.662965
C	Bicyclo[3.3.1]nonan-2-one	-426.621087
D	Bicyclo[3.3.1]nonane	-352.607967
E	Butane	-158.4580463
F	Butanone	-232.4705593
G	*N*,*N*-dimethylacetamide	-213.788638
H	*N*,*N*-dimethylethylamine	-287.830189

	1-Aza-9,10-benzobicyclo[3.3.2]decan-2-one **31** (Table 6)	[2]
A	1-Aza-9,10-benzobicyclo[3.3.2]decane	-560.363302
B	1-Aza-9,10-benzobicyclo[3.3.2]decan-2-one	-634.398988
C	9,10-Benzobicyclo[3.3.2]decan-2-one	-618.351237
D	9,10-Benzobicyclo[3.3.2]decane	-544.340686

	1-Azabicyclo[4.3.1]decan-10-one **32a** (Table 6)	[3]
A	1-Azabicyclo[4.3.1]decane	-407.921801
B	1-Azabicyclo[4.3.1]decan-10-one	-481.948955
C	Bicyclo[4.3.1]decan-10-one	-465.917739
D	Bicyclo[4.3.1]decane	-391.901293

[a] TA energy of 1-azaadamantan-2-one at B3LYP/6-31G(d)

[b] COSNAR energy of *N*,*N*-dimethylacetamide at B3LYP/6-31G(d)

Table S7. B3LYP/6-31G(d) TA and COSNAR results for 30, 31 and 32a in Table 6

Dataset (Table S5)		[1]	[2]	[3]
□□ΔE_{obs}/kJmol^{-1}	2625×((B+H)-(A+G))	3.63	15.40	37.80
□□ΔE_{corr}/kJmol^{-1}	2625×(C+E)-(D+F))	-1.59	5.15	-10.33
□□ΔE_{TA}/kJmol^{-1}	□ΔE_{obs}–ΔE_{corr}	5.22	10.25	48.12
RE_{TA}/kJmol^{-1}	–(76.03–E_{TA})	70.81	65.78	27.90
RE_{COSNAR}kJmol^{-1}	2625((B+D)-(A+C))	71.02	65.99	28.11
$Amidicity_{TA}$/%	100x(RE_{TA}/–76.03[a])	93.13	86.52	36.70
$Amidicity_{COSNAR}$/%	100x(RE_{COSNAR}/–77.51[b])	91.62	85.13	36.27

[a] TA energy of 1-azaadamantan-2-one at B3LYP/6-31G(d)

[b] COSNAR energy of *N*,*N*-dimethylacetamide at B3LYP/6-31G(d)

Table S8 B3LYP/6-31G(d,p) structures for strain enthalpies, ΔH^{RS} in Table 1

Butanone (Table S10, [1]F)
2-Butanol

H	2.107388	-1.021718	-0.451484
C	2.028675	-0.060589	0.062713
H	2.177488	-0.240154	1.134012
H	2.844368	0.582676	-0.282541
C	0.666472	0.583943	-0.204531
H	0.554765	0.793992	-1.276185
H	0.595127	1.546942	0.316615
C	-0.514348	-0.284490	0.230653
H	-0.395822	-0.518767	1.303598
C	-1.859417	0.414033	0.025318
H	-2.689811	-0.232755	0.332981
H	-1.999897	0.666266	-1.030751
H	-1.921840	1.334979	0.615132
O	-0.441565	-1.490582	-0.536428
H	-1.151583	-2.073776	-0.239101

Cyclobutanone (Table S10, [1]C)
Cyclobutanol

H	-2.110040	0.317800	0.706980
C	-1.318928	0.181898	-0.034089
C	-0.406555	-1.067020	0.110886
C	-0.050069	1.068005	0.100398
C	0.789841	-0.181275	-0.285835
H	0.957109	-0.213752	-1.373691
H	-1.762359	0.250155	-1.032103
H	0.028759	1.965489	-0.520791
H	0.145637	1.331533	1.144583
H	-0.620136	-1.950793	-0.496379
H	-0.302379	-1.367566	1.158010
O	1.979126	-0.463538	0.422657
H	2.669994	0.129063	0.099374

Cyclopentanone (Table S10, [3]C)
Cyclopentanol

H	-2.058533	0.582564	0.958833
C	-1.420757	0.300465	0.116101
C	-0.245131	1.295213	-0.102555
C	1.034498	0.438363	-0.228413
C	0.517271	-0.978489	-0.536181
C	-0.756598	-1.077231	0.316783
H	-2.061686	0.275712	-0.772693
H	-0.117076	1.985418	0.735172
H	-0.398212	1.899437	-1.002133
H	1.709821	0.815983	-1.010535
H	1.262374	-1.753305	-0.320084
H	0.268630	-1.053256	-1.603483
H	-0.474384	-1.210582	1.366496
H	-1.405821	-1.912273	0.035922
O	1.687292	0.486503	1.045928
H	2.458313	-0.094522	1.000840

Cyclohexanone ((Table S10, [4]C)
Cyclohexanol

C	1.276301	0.030790	0.246583
C	-0.912052	1.306993	0.229475
C	-0.930526	-1.229237	0.234365
C	-1.656440	0.043236	-0.227464
C	0.537372	-1.229626	-0.221407
C	0.555703	1.293516	-0.224370
H	-0.954650	1.374749	1.325900
H	-0.971677	-1.291201	1.331178
H	-1.723862	0.041249	-1.324488
H	0.592479	-1.267233	-1.317646
H	0.611464	1.326623	-1.320705
H	1.294842	0.034091	1.351993
H	-1.411978	2.203821	-0.154239
H	-1.441611	-2.121768	-0.144810
H	-2.686323	0.050954	0.149134
H	1.052777	-2.124801	0.154053
H	1.090942	2.174187	0.147200
O	2.607362	0.089898	-0.263901
H	3.069877	-0.706240	0.029149

2-Acetylcyclobutanone ((Table S10, [5]C)
2-Acetylcyclobutanol

H	-2.405244	0.990236	-0.399681
C	-1.595593	0.312133	-0.677344
C	-0.380014	0.240340	0.276288
C	-0.636114	0.764492	-1.811142
H	-2.007514	-0.686423	-0.840770
H	-0.798053	0.370190	-2.818645
H	-0.547259	1.854179	-1.857007
H	-0.190295	1.196003	0.778898
C	-0.246633	-0.916722	1.244738
O	-1.001326	-1.872337	1.210723
C	0.916544	-0.834788	2.215447
H	1.829164	-0.526223	1.693466
H	1.061855	-1.794388	2.713741
H	0.709325	-0.064628	2.968606
C	0.536450	0.181136	-0.980159
H	0.729873	-0.865289	-1.260371
O	1.738301	0.906420	-0.838765
H	2.286537	0.745668	-1.618023

7-Acetamido-2-thiabicyclo[3.2.0]heptan-6-one (Table S10,[10]C)
7-Acetamido-6-hydroxy-2-thiabicyclo[3.2.0]heptane

C	-0.689533	0.993489	0.405464
C	0.616146	0.159731	0.556952
C	-1.467142	-0.131877	1.154736
H	-0.677858	1.993078	0.844733
H	-1.578984	0.091580	2.219708
H	1.179310	0.497383	1.429965
S	-1.401920	1.053717	-1.292911
C	-2.799301	-0.487134	0.463221
H	-3.638713	-0.488789	1.167610
C	-3.053935	0.533820	-0.660289
H	-3.631643	0.122139	-1.491573
C	-0.234552	-1.071091	0.931239
H	-0.403925	-1.724654	0.062187
O	0.283510	-1.788909	2.026640
H	-0.242379	-2.590007	2.147685
N	1.548495	0.072391	-0.533199
H	1.191353	-0.224310	-1.430691
C	2.840160	0.536838	-0.447062
C	3.642259	0.407560	-1.733886
H	4.628159	0.843161	-1.575287
H	3.146423	0.924263	-2.562994
H	3.755232	-0.644858	-2.015113
O	3.309081	1.000145	0.582747
H	-2.740010	-1.493945	0.033841
H	-3.580231	1.416279	-0.283725

Table S9 B3LYP/6-31G(d,p) structures for hydrogenation enthalpies, ΔH^{obs} in Table 1 and Table 2 and Eq. 7

H_2

H	0.000000	0.000000	0.371403
H	0.000000	0.000000	-0.371403

3a Table S10 [1]B

3a + H_2 Azetidine-2-ol

H	0.668854	-0.200393	1.500113
C	0.706007	-0.161323	0.394786
C	-0.230581	0.938744	-0.175342
C	-1.232100	-0.213105	-0.429732
H	-2.005721	-0.271251	0.350094
H	-1.721505	-0.254578	-1.408886
H	0.179264	1.354678	-1.098152
H	-0.541215	1.741508	0.496912
O	2.046136	-0.214763	-0.040077
H	2.535343	0.472313	0.432787
N	-0.111841	-1.166924	-0.267878
H	-0.292641	-2.024905	0.245373

3b Table S10 [2]B

3b + H_2 *N*-Methylazetidine-2-ol

H	2.139101	0.671234	-0.444271
C	1.240058	0.044798	-0.403838
H	1.538545	-0.995948	-0.202743
C	0.229871	0.162959	-1.572359
H	0.338632	1.083076	-2.151548
H	0.143515	-0.696263	-2.240466
N	0.184450	0.547217	0.494232
C	0.093937	0.100478	1.870678
H	0.976529	0.449170	2.417714
H	0.026709	-0.993323	1.973095
H	-0.789035	0.542465	2.343575
C	-0.858921	0.244282	-0.469134
H	-1.637522	1.018785	-0.560390
O	-1.471878	-1.015234	-0.193066
H	-2.153991	-1.163696	-0.861478

4a Table S10 [3]B

4a + H_2 Pyrrolidin-2-ol

C	-0.185596	0.353361	1.037666
H	-0.120068	1.442155	1.159954
H	-0.553562	-0.070052	1.976690
C	1.171750	-0.206792	0.588405
H	1.193538	-1.292534	0.724682
H	2.023301	0.228101	1.118541
C	1.166294	0.128659	-0.908097
N	-0.229164	-0.103552	-1.280050
H	-0.542096	0.347783	-2.127487
H	1.487704	1.174324	-1.061604
H	1.842551	-0.511193	-1.487460
C	-1.115511	0.022147	-0.150818
O	-1.794127	-1.229353	0.019701
H	-2.475398	-1.095254	0.693605
H	-1.869617	0.812202	-0.303728

5a Table S10 [4]B

5a + H_2 Piperidine-2-ol

H	0.685273	1.532846	-1.249270
C	0.762922	1.389542	-0.152750
H	1.234728	2.289960	0.255350
C	1.630899	0.157212	0.124084
H	2.598784	0.262841	-0.380132
H	1.823495	0.100066	1.202117
C	0.912712	-1.118742	-0.341775
C	-0.502060	-1.192355	0.253790
H	-1.048278	-2.052413	-0.155615
H	-0.457672	-1.308577	1.342734
N	-0.541450	1.225630	0.489401
H	-1.110067	2.061395	0.380720
H	0.844864	-1.112577	-1.439143
H	1.488752	-2.010719	-0.071087
C	-1.282535	0.093402	-0.032880
H	-1.436583	0.172913	-1.134245
O	-2.542982	0.127758	0.619064
H	-3.060803	-0.618183	0.289636

3c Table S10 [5]B

3c + H_2 *N*-Acetylazetidine-2-ol

N	-0.435501	0.140033	0.135077
C	-0.228523	-1.906737	0.544018
H	0.253421	-2.392354	1.394872
H	-0.598568	-2.658910	-0.155448
C	-1.260894	-0.799363	0.897465
H	-2.270906	-0.928209	0.497040
H	-1.331424	-0.546081	1.960187
C	-0.512641	1.508638	0.116432
O	-1.444086	2.091245	0.655477
C	0.622583	2.217031	-0.602496
H	1.483446	2.314470	0.069896
H	0.287591	3.218257	-0.874845
H	0.942999	1.666279	-1.489635
C	0.616076	-0.810688	-0.173205
H	1.579374	-0.581641	0.311025
O	0.794296	-0.945142	-1.568634
H	1.502757	-1.586828	-1.717225

3c + H_2 *N*-1-Hydroxyethylazetidine

C	0.661561	-1.229559	-0.380809
O	1.610431	-1.202515	-1.129786
N	-0.039100	-0.233180	0.288487
C	-0.253019	-2.322885	0.209034
H	0.237834	-2.987186	0.923808
H	-0.772862	-2.914205	-0.547438
C	-1.065541	-1.150392	0.821014
H	-2.051627	-0.998870	0.372430
H	-1.143834	-1.133953	1.912816
C	-0.144739	1.182473	0.067932
H	-0.510877	1.624905	1.009010
C	1.201769	1.799364	-0.302956
H	1.588698	1.345675	-1.216132
H	1.930054	1.645830	0.498100
H	1.083113	2.877823	-0.453865
O	-1.125364	1.373165	-0.956534
H	-1.206498	2.323512	-1.115111

1 (Eq 7.)

H	2.752886	0.325475	0.013267
C	1.778495	0.812167	-0.000191
H	1.691603	1.458301	0.879261
H	1.710524	1.444709	-0.891167
C	0.728631	-0.293797	-0.003205
O	1.065813	-1.473540	0.006336
N	-0.595891	0.083784	-0.022312

C	-1.080637	1.451267	0.007835
H	-1.603055	1.667390	0.950563
H	-1.790532	1.620282	-0.812160
H	-0.266072	2.164350	-0.100841
C	-1.624869	-0.945200	0.002403
H	-2.232255	-0.865758	0.913563
H	-1.137111	-1.917827	-0.024786
H	-2.290825	-0.841552	-0.863359

1+H_2 (Eq. 7)

H	-0.139631	-0.536988	-2.610171
C	-0.109288	-0.716302	-1.528938
H	-1.006473	-1.277685	-1.254704
H	0.769334	-1.338085	-1.327385
C	-0.039748	0.614469	-0.760394
H	0.846531	1.170809	-1.108170
O	-1.220707	1.378847	-0.989441
H	-1.334801	1.459803	-1.944961
N	0.101141	0.512512	0.680859
C	1.429139	0.123828	1.117579
H	2.182137	0.760491	0.640918
H	1.690830	-0.931416	0.904405
H	1.507793	0.265584	2.200885
C	-0.955585	-0.233444	1.352451
H	-0.877338	-1.329933	1.232314
H	-1.923741	0.093466	0.969484
H	-0.919578	-0.015954	2.425268

Table S10 B3LYP/6-31G(d,p) Enthalpy Structures for TA-COSNAR data in Table 1

[1]A Azetidine

H	-0.189520	1.427238	1.052381
C	-0.150177	1.053482	0.017135
H	-0.165640	1.912761	-0.663319
C	0.968911	0.000320	-0.170359
H	1.788811	0.000018	0.550803
H	1.375958	0.001053	-1.184126
N	-1.147344	-0.000059	-0.295409
H	-1.977724	-0.000688	0.292015
C	-0.149723	-1.053545	0.015847
H	-0.164663	-1.912019	-0.665577
H	-0.188893	-1.428561	1.050607

[1]B β-propiolactam

H	0.587921	0.561767	-1.654203
C	0.101183	0.696706	-0.682455
H	-0.346023	1.695162	-0.632834
C	-0.830506	-0.468008	-0.240713
H	-0.899096	-1.307784	-0.935375
H	-1.831053	-0.175104	0.084392
C	0.175873	-0.682974	0.919255
O	0.280155	-1.438226	1.856002
N	0.950479	0.360916	0.466490
H	1.811066	0.757545	0.819442

[1]C Cyclobutanone

H	-1.119936	0.000128	1.460652
C	-0.136104	-0.000738	0.986457
H	0.626262	-0.002368	1.768208
C	0.031008	-1.110650	-0.096597
H	-0.800405	-1.811467	-0.223325
H	0.958257	-1.690475	-0.031693
C	0.095702	0.000905	-1.158997
O	0.144592	0.001929	-2.361281
C	0.033822	1.110785	-0.094587
H	0.962550	1.688203	-0.028691
H	-0.795942	1.813747	-0.220145

[1]D Cyclobutane

H	1.005326	-1.168675	-1.001451
C	0.767539	-0.126279	-0.765443
H	1.392211	0.519889	-1.389407
C	-0.765283	0.124466	-0.767410
H	-1.388394	-0.523329	-1.391309
H	-1.002484	1.166373	-1.006378
C	0.765824	0.126205	0.767078
H	1.003026	1.168610	1.003764
H	1.389153	-0.519890	1.392474
C	-0.767020	-0.124482	0.765618
H	-1.005178	-1.166332	1.004476
H	-1.391601	0.523444	1.387989

[1]E Butane

H	1.167781	0.876440	0.463275
C	0.514954	-0.000750	0.568827
H	1.167096	-0.878224	0.461494
C	-0.122871	-0.001896	1.961041
H	0.634567	-0.002483	2.751629
H	-0.755078	-0.885554	2.105413
C	-0.514915	0.000804	-0.568819
H	-1.167035	0.878276	-0.461481
H	-1.167784	-0.876357	-0.463233
C	0.122842	0.001862	-1.961030
H	0.755007	-0.881604	-2.106874
H	-0.634637	0.002648	-2.751587
H	-0.755190	0.881440	2.106803
H	0.755263	0.885398	-2.105458

[1]F Butanone

H	0.309940	0.010590	2.755729
C	-0.364624	-0.017091	1.895105
H	-0.962032	-0.930853	1.953785
C	0.260270	-0.019207	-1.996097
H	0.811099	-0.961846	-2.098728
H	-0.464901	0.064724	-2.806495
C	-0.457786	0.021393	-0.656957
O	-1.672225	0.037980	-0.585434
C	0.421994	0.037015	0.588217
H	1.132226	-0.798673	0.514197
H	1.045641	0.941630	0.539909
H	-1.056406	0.825768	1.968061
H	0.996805	0.788571	-2.071293

[2]A *N*-Methylazetidine

H	0.978336	-1.398605	-0.248661
C	-0.042536	-1.049776	-0.486308
H	-0.699068	-1.922658	-0.580277
C	-0.037392	0.000606	-1.622343
H	0.818206	0.002949	-2.299715
H	-0.964190	-0.001273	-2.199760
N	-0.524559	-0.001446	0.437837
C	-0.028587	-0.000842	1.797081
H	1.077858	0.000791	1.857962
H	-0.396395	-0.885863	2.327738
H	-0.398855	0.883258	2.327751
C	-0.047214	1.049824	-0.485331
H	0.972059	1.403086	-0.247432
H	-0.707665	1.919948	-0.578540

[2]B *N*-Methyl-β-propiolactam

C	-0.722646	-0.000689	0.980403
O	-1.841273	-0.000988	1.443999
N	-0.262998	-0.001181	-0.316165
C	0.724218	0.000417	1.527986
H	0.990392	-0.892357	2.098117
H	0.988787	0.893590	2.098259
C	1.161147	0.000678	0.035090
H	1.700216	0.895749	-0.297552
H	1.702701	-0.893061	-0.297194
C	-0.961937	-0.000665	-1.575705
H	-2.032168	0.001744	-1.355772
H	-0.725271	-0.892074	-2.170119
H	-0.721167	0.888835	-2.171347

[2]C 2-Methylcyclobutanone

H	-2.270763	-0.432232	1.012052
C	-1.672140	-0.380901	0.098052
H	-2.324245	-0.595925	-0.756202
C	-0.314479	-1.145715	0.056998
H	-0.271527	-2.019521	-0.595964
H	0.026618	-1.433815	1.055435
C	0.413452	0.138494	-0.459331
H	0.513604	0.104788	-1.553607

C	1.719740	0.600300	0.175005
H	2.544555	-0.072402	-0.081185
H	1.635854	0.634181	1.266333
H	1.978333	1.605920	-0.170071
C	-0.870357	0.914156	-0.108636
O	-1.108645	2.082673	0.061123

[2]D Methylcyclobutane

H	-0.709436	-0.559790	-1.973153
C	-0.561050	0.059928	-1.082061
C	0.436848	-0.445954	0.000000
C	-1.673834	0.064452	0.000000
C	-0.561050	0.059928	1.082061
H	-0.709436	-0.559790	1.973153
H	-0.309189	1.077622	1.405383
H	-0.309189	1.077622	-1.405383
H	-2.382686	0.898674	0.000000
H	-2.241300	-0.872505	0.000000
H	0.445956	-1.544318	0.000000
C	1.864688	0.081243	0.000000
H	2.416669	-0.258019	-0.885766
H	2.416669	-0.258019	0.885766
H	1.876338	1.178924	0.000000

[3]A Pyrrolidine

H	-1.225035	0.650392	-1.332528
C	-0.157017	0.468513	-1.156064
H	0.379891	0.777852	-2.057368
C	0.071179	-1.021168	-0.777836
H	1.032385	-1.375937	-1.164829
H	-0.701753	-1.672865	-1.197091
C	0.070899	-1.021225	0.777812
H	1.031685	-1.376712	1.165172
H	-0.702634	-1.672473	1.196724
C	-0.156692	0.468569	1.156085
H	0.380611	0.777831	2.057200
H	-1.224594	0.650703	1.333004
N	0.257858	1.278049	-0.000075
H	1.275989	1.333755	-0.000208

[3]B γ-Butyrolactam

C	-0.906774	-0.002639	-0.007677
O	-2.124381	0.012824	-0.039932
C	0.008716	-1.224566	0.138813
H	-0.069967	-1.576698	1.174623
H	-0.330025	-2.036571	-0.507668
C	1.414415	-0.693454	-0.188467
H	1.624417	-0.824669	-1.254483
H	2.212050	-1.186701	0.371743
C	1.326774	0.817726	0.133603
N	-0.085574	1.095675	-0.077114
H	-0.484428	2.021561	-0.022954
H	1.631321	1.025584	1.170397
H	1.957279	1.422508	-0.526230

[3]C Cyclopentanone

C	-0.118901	1.238826	0.030982
H	-1.162301	1.579618	0.086375
H	0.503428	2.055453	0.406358
C	0.227877	0.738878	-1.381120
H	1.312285	0.791540	-1.538235
H	-0.243431	1.324910	-2.174895
C	-0.228014	-0.739227	-1.380743
H	-1.312315	-0.791525	-1.538006
H	0.243001	-1.325697	-2.174331
C	0.118755	-1.238701	0.031465
H	1.161723	-1.580716	0.087006
H	-0.504521	-2.054325	0.407591
C	0.000662	0.000319	0.929032
O	0.001752	0.000648	2.140013

[3]D Cyclopentane

H	-1.557640	1.660996	-0.136803
C	-0.862744	0.915358	0.263634
C	-1.160897	-0.514720	-0.214431
C	0.143499	-1.292115	0.080690
C	1.284634	-0.228532	0.062715
C	0.590587	1.132973	-0.191413
H	-0.924706	0.964852	1.359003
H	-1.355378	-0.502391	-1.294601
H	-2.038805	-0.960250	0.265569
H	0.085325	-1.766165	1.066311
H	0.311825	-2.095775	-0.642660
H	2.038147	-0.445547	-0.700510
H	1.808335	-0.217965	1.024299
H	0.602937	1.366455	-1.263458
H	1.085397	1.963452	0.323043

[4]A Piperidine

C	-0.688211	-1.279521	-0.228753
C	-0.744201	1.247740	-0.227900
C	-1.456473	-0.032415	0.234234
C	0.726987	1.231695	0.201227
C	0.780367	-1.198327	0.201745
H	-0.728347	-1.353008	-1.322677
H	-0.788241	1.320100	-1.321678
H	-1.515659	-0.034251	1.332354
H	0.775503	1.292165	1.307724
H	0.829571	-1.254744	1.308395
H	-1.145121	-2.189295	0.179016
H	-1.240921	2.135812	0.181048
H	-2.488726	-0.055722	-0.134999
H	1.248051	2.111523	-0.193080
H	1.340923	-2.054374	-0.190672
N	1.379845	0.030302	-0.324401
H	2.371012	0.052330	-0.100340

[4]B δ-Valerolactam

H	1.279490	1.476877	-1.206722
C	1.037473	1.287066	-0.149044
H	1.385569	2.156194	0.420552
C	1.755505	0.020176	0.314541
H	2.813066	0.089021	0.038432
H	1.707879	-0.049450	1.408693
C	1.096333	-1.213196	-0.310006
C	-0.372649	-1.300648	0.125227
H	-0.930715	-2.046657	-0.446531
H	-0.434342	-1.609131	1.177485
C	-1.148248	0.009326	0.019957
O	-2.372300	0.035945	-0.007310
N	-0.407868	1.163857	0.028315
H	-0.973963	1.996692	-0.073888
H	1.157326	-1.140192	-1.404102
H	1.630132	-2.126726	-0.026925

[4]C Cyclohexanone

C	-1.013283	-0.281366	1.266882
C	-1.013165	-0.281418	-1.266787
C	-1.787798	0.108520	-0.000000
C	0.397711	0.343686	-1.286356
C	0.397682	0.343499	1.286311
H	-0.921596	-1.374758	1.312295
H	-0.921185	-1.374810	-1.311944
H	-1.969114	1.192815	-0.000046
H	0.302561	1.435711	-1.382836
H	0.302639	1.435552	1.382708
H	-1.562972	0.021982	2.164861
H	-1.562911	0.021554	-2.164863
H	-2.773333	-0.371330	-0.000033
H	0.995725	-0.012252	-2.129311
H	0.995749	-0.012426	2.129225
C	1.164230	0.065228	-0.000043
O	2.310566	-0.342265	-0.000063

[4]D Cyclohexane

H	2.498361	-0.000003	-0.146292
C	1.467439	-0.000002	0.228749
C	-0.733416	1.269786	0.229263
C	-0.733416	-1.269786	0.229263
C	-1.467439	0.000002	-0.228749
C	0.733416	-1.269786	-0.229263
C	0.733416	1.269786	-0.229263
H	-0.767964	1.329877	1.326741
H	-0.767964	-1.329877	1.326741
H	-1.535672	0.000002	-1.326341
H	0.767964	-1.329877	-1.326741
H	0.767964	1.329877	-1.326741
H	1.535672	-0.000002	1.326341
H	-1.248138	2.162418	-0.146637
H	-1.248138	-2.162418	-0.146637
H	-2.498361	0.000003	0.146292
H	1.248138	-2.162418	0.146637
H	1.248138	2.162418	0.146637

[5]A *N*-Acetylazetidine

C	0.263622	0.849015	-1.394431
H	1.094990	0.653795	-2.079599
H	-0.657735	0.939199	-1.980663
C	0.496324	1.960954	-0.330558
H	-0.235918	2.770038	-0.336611
H	1.500606	2.388078	-0.338820
C	0.274425	0.883899	0.769930
H	1.115603	0.718560	1.453568
H	-0.639056	1.013730	1.364661
N	0.156821	-0.118175	-0.298860
C	-0.343489	-1.385195	-0.356125
O	-0.590101	-1.924912	-1.429255
C	-0.560964	-2.060279	0.989687
H	0.300271	-1.933671	1.653161
H	-0.740046	-3.121655	0.818808
H	-1.435353	-1.633379	1.495107

[5]B *N*-Acetyl-β-propiolactam

C	0.766090	-0.945262	-0.267744
O	1.807686	-0.826271	-0.861991
N	-0.204561	-0.006036	0.118033
C	-0.047698	-2.088229	0.364824
H	0.459679	-2.587970	1.193246
H	-0.394389	-2.835074	-0.353094
C	-1.084035	-0.998866	0.763344
H	-2.063682	-1.074078	0.286201
H	-1.206624	-0.826676	1.835030
C	-0.379081	1.372306	-0.010527
O	-1.373695	1.898582	0.454372
C	0.723824	2.099990	-0.743290
H	1.687630	1.939833	-0.251149
H	0.481597	3.162454	-0.764882
H	0.827260	1.715295	-1.762374

[5]C *2*-Acetylcyclobutanone

H	-2.106541	1.281243	-0.708701
C	-1.390403	0.469277	-0.843378
C	-0.260629	0.410329	0.216993
C	-0.350882	0.685811	-1.985454
H	-1.923349	-0.481006	-0.903656
H	-0.327767	-0.063279	-2.783944
H	-0.357434	1.678651	-2.448491
H	-0.185258	1.281889	0.879551
C	0.765007	0.532202	-0.948644
O	1.966037	0.481731	-0.991510
C	-0.116843	-0.867532	1.038479
O	-0.888086	-1.797511	0.904397
C	1.072726	-0.907234	1.972308
H	1.983458	-0.652973	1.417882
H	1.162169	-1.896748	2.422306
H	0.957795	-0.154850	2.761863

[5]D acetylcyclobutane

C	-1.515131	1.150593	-0.971897
H	-1.291639	1.555969	-1.963650
H	-2.474757	1.556217	-0.639934
C	-0.309337	1.302703	-0.007486
H	-0.630175	1.384082	1.035689
H	0.421407	2.088988	-0.215852
C	0.101127	-0.171810	-0.358816
H	0.866848	-0.173744	-1.143653
C	-1.326517	-0.388190	-0.916550
H	-1.416472	-0.947652	-1.851742
H	-1.951938	-0.861953	-0.155671
C	0.550602	-1.021766	0.814763
O	-0.236399	-1.690313	1.460681
C	2.025051	-0.957841	1.172727
H	2.617044	-1.446834	0.389519
H	2.202579	-1.460217	2.124723
H	2.367706	0.081768	1.227150

[6]A *N*-Ethyl-β-propiolactam

C	1.044004	-1.111040	0.563582
O	2.232632	-1.090659	0.795628
N	0.133294	-0.105714	0.331573
C	-0.054629	-2.188914	0.413987
H	-0.238127	-2.771678	1.319356
H	0.087696	-2.862817	-0.433898
C	-1.024048	-0.996371	0.172294
H	-1.486196	-0.961869	-0.820833
H	-1.797112	-0.858710	0.937809
C	0.279175	1.334252	0.314149
H	1.303283	1.532881	0.645025
H	-0.397286	1.778117	1.058027
C	0.027337	1.954800	-1.063195
H	0.732161	1.560652	-1.800727
H	0.146216	3.042063	-1.018387

H	-0.988401	1.745004	-1.414391

[6]C 2-Ethylcyclobutanone

C	0.683323	-1.109664	-0.476965
O	1.851804	-1.071350	-0.772514
C	-0.260562	-2.235404	-0.028387
H	0.156034	-2.957820	0.679388
H	-0.669736	-2.783623	-0.884523
C	-1.213541	-1.126772	0.511999
H	-2.265020	-1.213437	0.231634
H	-1.145441	-1.018005	1.598233
C	-0.388167	-0.028186	-0.235809
H	-0.863460	0.220242	-1.196154
C	0.027970	1.253473	0.487525
H	0.544814	0.983807	1.417688
H	-0.876221	1.800877	0.784312
C	0.932896	2.150575	-0.364857
H	1.841487	1.616138	-0.653806
H	1.220984	3.052485	0.184244
H	0.422837	2.466666	-1.282009

[7]A *N*-Ethylazetidine

C	1.221821	-0.974388	0.056777
C	0.679585	1.043676	-0.150652
C	2.042488	0.336220	0.034680
H	2.502348	0.560316	0.999523
H	2.781072	0.453700	-0.760352
H	0.463236	1.240020	-1.215953
H	0.484366	1.957120	0.422442
H	1.188632	-1.449819	-0.939610
H	1.471008	-1.738363	0.802574
N	0.013468	-0.177510	0.356865
C	-1.244044	-0.589653	-0.241932
H	-1.453846	-1.612056	0.098137
H	-1.171013	-0.633740	-1.348833
C	-2.393702	0.331869	0.160922
H	-3.336277	-0.006350	-0.281507
H	-2.217000	1.358131	-0.179196
H	-2.505229	0.351948	1.249044

[7]C Ethylcyclobutane

H	-3.414440	-0.011831	0.361707
C	-2.472780	-0.334510	-0.094463
H	-2.269729	-1.354565	0.250356
H	-2.625843	-0.377530	-1.179076
C	-1.322401	0.612993	0.263032
H	-1.210071	0.661352	1.355287
H	-1.572160	1.632624	-0.062415
C	0.011295	0.205103	-0.354676
C	0.727207	-1.084989	0.144231
C	1.296480	0.999062	0.015706
C	2.081126	-0.339460	0.006903
H	2.831290	-0.496485	0.787317
H	2.548035	-0.527460	-0.965238
H	-0.090171	0.163369	-1.447895
H	1.623352	1.794154	-0.661890
H	1.223732	1.414415	1.027760
H	0.587433	-2.008413	-0.426020
H	0.486230	-1.286098	1.194923

[8]A *N*-(1-hydroxethyl)azetidine

C	1.429287	-0.861927	0.089098
C	0.846324	1.160852	-0.011999
C	2.223579	0.465673	0.104338
H	2.710119	0.656273	1.063302
H	2.935392	0.632976	-0.705980
H	0.607556	1.423810	-1.057392
H	0.648923	2.032221	0.621809
H	1.384496	-1.308281	-0.918717
H	1.699735	-1.641576	0.806517
N	0.208635	-0.098243	0.432668
C	-1.033565	-0.501169	-0.175588
H	-0.929018	-0.559842	-1.284839
C	-2.155227	0.474256	0.172601
H	-3.098350	0.142783	-0.274366
H	-1.944035	1.480513	-0.203510
H	-2.273411	0.516602	1.258175
O	-1.300430	-1.805291	0.330868
H	-1.960011	-2.209631	-0.246985

[8]B *N*-(1-Hydroxyethyl)-β-propiolactam

C	0.661561	-1.229560	-0.380809
O	1.610432	-1.202515	-1.129787
N	-0.039100	-0.233181	0.288487
C	-0.253020	-2.322886	0.209034
H	0.237834	-2.987187	0.923808
H	-0.772862	-2.914206	-0.547439
C	-1.065541	-1.150392	0.821014
H	-2.051627	-0.998871	0.372431
H	-1.143834	-1.133954	1.912816
C	-0.144739	1.182473	0.067932
H	-0.510878	1.624905	1.009011
C	1.201769	1.799365	-0.302956
H	1.588699	1.345675	-1.216132
H	1.930055	1.645831	0.498100
H	1.083114	2.877823	-0.453865
O	-1.125364	1.373166	-0.956534
H	-1.206498	2.323512	-1.115111

[8]C 2-(1-Hydroxyethyl)-cyclobutanone

H	-2.128891	-0.868754	-1.188467
C	-1.297092	-1.083728	-0.516810
C	-0.172579	-0.003271	-0.459733
C	-0.269310	-2.150490	-1.004254
H	-1.696385	-1.309753	0.475242
H	-0.228389	-3.112615	-0.485268
H	-0.309865	-2.340614	-2.082918
H	-0.189499	0.633837	-1.354771
C	0.838476	-1.150611	-0.647126
O	2.025675	-1.249221	-0.458924
C	1.222936	1.748402	0.717788
H	2.117637	1.125871	0.627725
H	1.315713	2.357356	1.625104
H	1.175602	2.423953	-0.142579
C	-0.032226	0.878650	0.774672
H	0.028273	0.222607	1.660456
O	-1.225749	1.663351	0.833950
H	-1.174328	2.215029	1.625914

[8]D 1-Cyclobutylethanol

H	3.239683	-0.375147	-0.311724
C	2.290025	0.078863	-0.607425
H	2.431090	1.163419	-0.656424
H	2.026517	-0.285101	-1.605046
C	1.204534	-0.265647	0.404676
H	1.069434	-1.362773	0.421188

O	1.679814	0.182341	1.677258
H	0.999228	-0.025929	2.330853
C	-0.140940	0.372992	0.074316
C	-1.371834	0.013937	0.960021
C	-0.941784	-0.128887	-1.160520
C	-2.242299	0.003228	-0.324921
H	-2.993288	-0.785562	-0.423100
H	-2.731041	0.968788	-0.487524
H	-0.010888	1.461498	0.034080
H	-0.866423	0.447038	-2.087009
H	-0.711868	-1.177134	-1.384696
H	-1.651975	0.706827	1.759245
H	-1.277982	-0.992751	1.386751

[9]A *N*-Ethyl-2-hydroxyazetidine

N	-0.487637	0.005396	-0.150345
C	-0.426120	-2.044037	0.343046
H	-0.180784	-2.718646	1.165801
H	-0.712927	-2.613268	-0.543223
C	-1.383154	-0.866044	0.637383
H	-2.411362	-0.923549	0.263532
H	-1.410741	-0.613758	1.710512
C	0.604718	-0.948192	-0.024321
H	1.279348	-0.718422	0.825123
O	1.357408	-1.082282	-1.210457
H	2.245010	-1.378062	-0.971606
C	-0.296811	1.394370	0.235894
H	0.136479	1.474897	1.253628
H	-1.288804	1.860724	0.283435
C	0.578254	2.150771	-0.763093
H	1.576819	1.709796	-0.829965
H	0.685882	3.198607	-0.463842
H	0.134421	2.111698	-1.761502

[9]B *N*-Acetyl-2-hydroxyazetidine

N	-0.432490	0.130711	0.161516
C	-0.269377	-1.924084	0.542861
H	0.206311	-2.449600	1.373276
H	-0.666910	-2.643006	-0.175537
C	-1.264710	-0.795641	0.932839
H	-2.287220	-0.892715	0.555724
H	-1.303263	-0.553374	2.000013
C	-0.508864	1.497944	0.111640
O	-1.433882	2.095740	0.645562
C	0.619487	2.187631	-0.635871
H	1.494350	2.284683	0.018460
H	0.288933	3.188403	-0.914810
H	0.915918	1.621363	-1.521656
C	0.599727	-0.840395	-0.160757
H	1.564691	-0.637889	0.330197
O	0.788397	-0.978734	-1.553842
H	1.688902	-1.291038	-1.709615

[9]C 2-Acetylcyclobutanol

H	-2.405244	0.990236	-0.399681
C	-1.595593	0.312133	-0.677344
C	-0.380014	0.240340	0.276288
C	-0.636114	0.764492	-1.811142
H	-2.007514	-0.686423	-0.840770
H	-0.798053	0.370190	-2.818645
H	-0.547259	1.854179	-1.857007
H	-0.190295	1.196003	0.778898
C	-0.246633	-0.916722	1.244738
O	-1.001326	-1.872337	1.210723
C	0.916544	-0.834788	2.215447
H	1.829164	-0.526223	1.693466
H	1.061855	-1.794388	2.713741
H	0.709325	-0.064628	2.968606
C	0.536450	0.181136	-0.980159
H	0.729873	-0.865289	-1.260371
O	1.738301	0.906420	-0.838765
H	2.286537	0.745668	-1.618023

[9]D 2-Ethylcyclobutanol

H	-3.378718	0.131210	0.347086
C	-2.430902	-0.168484	-0.112020
H	-2.207217	-1.191806	0.205245
H	-2.576431	-0.190929	-1.197719
C	-1.297542	0.791272	0.269036
H	-1.205079	0.841926	1.363168
H	-1.549372	1.808853	-0.060003
C	0.049722	0.393785	-0.324945
C	0.769798	-0.873448	0.184855
C	1.334747	1.193681	0.036304
C	2.125878	-0.141295	0.005169
H	2.909479	-0.301481	0.751840
H	2.526514	-0.347959	-0.991932
H	-0.028642	0.307054	-1.416721
H	1.648014	1.987661	-0.646454
H	1.276258	1.608051	1.048905
H	0.554237	-1.025980	1.255180
O	0.500756	-2.043713	-0.561997
H	0.978501	-2.778396	-0.154998

[10]A 6-Acetamido-1-aza-3,3-dimethyl-4-thia bicyclo[3.2.0]heptane-2-carboxylic acid

N	-0.376742	-0.132839	-1.249776
C	0.724587	-0.615553	-0.372791
H	1.151723	-1.579281	-0.661034
C	1.557162	0.650401	-0.730299
H	2.320853	0.428523	-1.476414
C	3.558310	1.639027	0.310450
O	4.287045	1.289797	-0.606413
N	2.202538	1.387716	0.313984
H	1.648746	1.650983	1.117305
S	0.048002	-0.705888	1.339201
C	-1.632726	-1.142617	0.638380
C	-1.711948	-0.235786	-0.634897
H	-2.061548	0.755214	-0.322163
C	-2.726714	-0.780784	1.647573
H	-2.653849	0.265658	1.957715
H	-2.658569	-1.411699	2.538497
H	-3.704283	-0.937196	1.183305
C	-1.686514	-2.642469	0.300137
H	-1.512224	-3.235530	1.200814
H	-0.936507	-2.927595	-0.443232
H	-2.673860	-2.900951	-0.096213
C	-2.743485	-0.768623	-1.649109
O	-3.928857	-0.816117	-1.411119
O	-2.204124	-1.187856	-2.800727
H	-1.240389	-0.994886	-2.709035
C	4.060819	2.396178	1.528143
H	3.819682	1.860474	2.452391
H	3.600156	3.388213	1.585870
H	5.141393	2.507003	1.446647
C	0.252912	1.220178	-1.343897

H	-0.233953	1.957282	-0.692936
H	0.312366	1.619024	-2.360357

[10]B 6-Acetamidopenicillanic acid

C	0.274387	1.259950	-1.197145
O	-0.169513	2.353579	-1.414028
N	-0.360205	-0.013703	-1.209058
C	0.727465	-0.612902	-0.388861
H	1.111531	-1.564612	-0.759231
C	1.597484	0.657344	-0.667967
H	2.333913	0.481650	-1.457805
C	3.621773	1.598706	0.330354
O	4.316536	1.213125	-0.596942
N	2.267943	1.331830	0.391562
H	1.717815	1.687095	1.159996
S	0.017110	-0.768098	1.294999
C	-1.677482	-1.114513	0.558035
C	-1.730964	-0.172129	-0.697349
H	-2.098597	0.814632	-0.395057
C	-2.763914	-0.745188	1.571822
H	-2.664595	0.291974	1.904285
H	-2.715909	-1.397909	2.448221
H	-3.743310	-0.867597	1.100932
C	-1.771910	-2.602400	0.178983
H	-1.619583	-3.223327	1.064487
H	-1.022994	-2.886972	-0.566574
H	-2.761952	-2.823181	-0.230832
C	-2.711671	-0.687347	-1.764253
O	-3.891435	-0.815539	-1.537740
O	-2.164781	-0.992999	-2.951036
H	-1.215183	-0.770907	-2.897314
C	4.162758	2.428568	1.478671
H	5.189427	2.120277	1.679143
H	3.566597	2.338825	2.390936
H	4.179259	3.481766	1.178766

[10]C 7-Acetamido-3,3-dimethyl-2-thia bicyclo[3.2.0]heptan-6-one-4-carboxylic acid

C	0.065112	1.629684	-0.844412
O	-0.774000	2.487305	-0.926003
C	1.132072	-0.094689	-0.177380
H	2.035778	-0.660864	-0.404200
C	1.331446	1.450379	0.015321
H	2.223073	1.780724	-0.531364
C	2.477235	2.781039	1.726819
O	3.465855	2.939894	1.024709
N	1.392426	2.041953	1.312374
H	0.584265	1.953582	1.910582
S	0.137726	-0.892949	1.137652
C	-1.018636	-1.707754	-0.088484
C	-1.184789	-0.621679	-1.213380
H	-1.984933	0.059997	-0.903559
C	-2.335193	-2.019247	0.631756
H	-2.789091	-1.111558	1.038997
H	-2.167369	-2.719937	1.455633
H	-3.044028	-2.478005	-0.063309
C	-0.376243	-2.998242	-0.622947
H	-0.168831	-3.683911	0.202056
H	0.562055	-2.803336	-1.149213
H	-1.055993	-3.502543	-1.319478
C	2.345762	3.402832	3.105565
H	1.516106	2.996704	3.690471
H	2.200367	4.481615	2.991180
H	3.281082	3.252059	3.648728
C	-1.616222	-1.222606	-2.543878
O	-0.923346	-1.346482	-3.529569
O	-2.907740	-1.632132	-2.509888
H	-3.098689	-2.006919	-3.387048
C	0.125792	0.169614	-1.340835
H	0.568952	0.075473	-2.336896

[10]D7-Acetamido-3,3-dimethyl-2-thia bicyclo[3.2.0]heptane-4-carboxylic acid

C	1.633319	-0.582113	-0.268174
H	2.524132	-1.110980	-0.610971
C	1.919941	0.944903	-0.059377
H	2.977527	1.216492	-0.119413
C	1.586968	2.791055	1.511005
O	2.212574	3.564055	0.793799
N	1.359337	1.492356	1.153775
H	0.890994	0.849733	1.781132
S	0.794920	-1.561552	1.038494
C	-0.779746	-1.776021	0.032655
C	-0.796700	-0.481603	-0.850976
H	-1.088811	0.343360	-0.193270
C	-1.971317	-1.850788	0.994167
H	-2.054632	-0.945041	1.600835
H	-1.869695	-2.707381	1.667181
H	-2.903945	-1.973155	0.434583
C	-0.676534	-3.063678	-0.799168
H	-0.570146	-3.928016	-0.138368
H	0.183258	-3.047234	-1.472972
H	-1.576842	-3.206851	-1.406847
C	1.021183	3.211945	2.859069
H	1.851142	3.432189	3.537104
H	0.378640	2.457902	3.321879
H	0.454112	4.136645	2.728172
C	-1.824986	-0.558429	-1.967340
O	-1.623817	-0.958123	-3.093317
O	-3.046925	-0.138184	-1.555617
H	-3.639826	-0.239086	-2.320308
C	0.619562	-0.241670	-1.395797
H	0.753762	-0.778763	-2.336806
C	1.123550	1.229769	-1.369975
H	1.778650	1.471277	-2.210027
H	0.360350	2.006988	-1.285125

Table S11 B3LYP/6-31G(d,p) conformers and structures for hydrogenation enthalpies, ΔH^{obs} in Table 2

14_{eq}NHB

C	0.298707	1.334539	-1.151222
O	-0.148160	2.438912	-1.323582
N	-0.318431	0.074331	-1.177728
C	0.779504	-0.563080	-0.429416
H	1.148868	-1.501449	-0.846655
C	1.642446	0.720571	-0.676763
H	2.368982	0.577217	-1.480742
C	3.672166	1.617498	0.359591
O	4.376810	1.245805	-0.566576
N	2.317666	1.361317	0.402809
H	1.765119	1.711446	1.171578
S	0.105737	-0.793969	1.268082
C	-1.605814	-1.099669	0.556882
C	-1.675362	-0.140642	-0.698833
H	-2.082376	0.827000	-0.385366
C	-2.669740	-0.720881	1.591722
H	-2.543698	0.309967	1.933844
H	-2.621615	-1.383900	2.460431
H	-3.662027	-0.817127	1.140540
C	-1.732949	-2.583943	0.170988
H	-1.574132	-3.210308	1.051607
H	-1.004963	-2.874732	-0.591308
H	-2.736713	-2.792359	-0.215041
C	-2.659248	-0.673951	-1.734822
O	-3.860368	-0.637228	-1.573798
O	-2.072297	-1.213334	-2.819078
H	-2.796550	-1.523662	-3.389865
C	4.209437	2.419555	1.530554
H	5.214855	2.066806	1.763946
H	3.581191	2.353709	2.422882
H	4.282955	3.471562	1.235341

14_{ax}NHB

C	-0.494245	1.810562	-0.453206
H	-0.757589	2.842741	-0.205169
C	-0.878554	0.802020	0.685345
H	-1.595584	1.123684	1.438994
C	0.968395	1.449405	-0.059189
O	2.069792	1.560201	-0.534228
N	0.521912	0.807858	1.108046
C	1.044794	-0.422097	1.658269
H	2.128933	-0.419407	1.497035
C	0.405063	-1.622952	0.842474
S	-1.233427	-0.950278	0.195974
C	1.323965	-1.990481	-0.336843
H	2.247448	-2.452658	0.035284
H	1.601282	-1.117518	-0.932123
H	0.831478	-2.713038	-0.993316
C	0.121872	-2.869544	1.693475
H	1.054358	-3.278663	2.099802
H	-0.331588	-3.649439	1.075633
H	-0.558112	-2.653530	2.519416
N	-0.919507	1.573135	-1.791557
H	-0.807424	0.643058	-2.168252
C	-1.543049	2.548248	-2.540471
O	-1.754045	3.671230	-2.107897
C	-1.916089	2.130946	-3.951766
H	-1.177066	2.538075	-4.649124
H	-2.883491	2.570203	-4.199536
H	-1.961224	1.047116	-4.086510
C	0.719214	-0.487039	3.158670
O	-0.301431	-0.060725	3.633068
O	1.641841	-1.103244	3.939444
H	2.432077	-1.327867	3.428261

15_{eq}HB

C	0.274387	1.259950	-1.197145
O	-0.169513	2.353579	-1.414028
N	-0.360205	-0.013703	-1.209058
C	0.727465	-0.612902	-0.388861
H	1.111531	-1.564612	-0.759231
C	1.597484	0.657344	-0.667967
H	2.333913	0.481650	-1.457805
C	3.621773	1.598706	0.330354
O	4.316536	1.213125	-0.596942
N	2.267943	1.331830	0.391562
H	1.717815	1.687095	1.159996
S	0.017110	-0.768098	1.294999
C	-1.677482	-1.114513	0.558035
C	-1.730964	-0.172129	-0.697349
H	-2.098597	0.814632	-0.395057
C	-2.763914	-0.745188	1.571822
H	-2.664595	0.291974	1.904285
H	-2.715909	-1.397909	2.448221
H	-3.743310	-0.867597	1.100932
C	-1.771910	-2.602400	0.178983
H	-1.619583	-3.223327	1.064487
H	-1.022994	-2.886972	-0.566574
H	-2.761952	-2.823181	-0.230832
C	-2.711671	-0.687347	-1.764253
O	-3.891435	-0.815539	-1.537740
O	-2.164781	-0.992999	-2.951036
H	-1.215183	-0.770907	-2.897314
C	4.162758	2.428568	1.478671
H	5.189427	2.120277	1.679143
H	3.566597	2.338825	2.390936
H	4.179259	3.481766	1.178766

15_{ax}HB

C	-0.549129	1.684619	-0.440502
H	-0.898996	2.695371	-0.208425
C	-0.909608	0.651105	0.683782
H	-1.680886	0.953046	1.394704
C	0.914838	1.442370	0.014887
O	2.020469	1.636154	-0.411199
N	0.478166	0.756184	1.179977
C	1.091760	-0.465115	1.697763
H	2.167661	-0.388779	1.503166
C	0.527871	-1.688584	0.872611
S	-1.149384	-1.108695	0.212588
C	1.470580	-1.980441	-0.309485
H	2.418735	-2.384133	0.065412
H	1.694196	-1.086208	-0.895833
H	1.028303	-2.725764	-0.976016
C	0.293066	-2.980118	1.666825
H	1.235120	-3.342498	2.083497
H	-0.108278	-3.747484	0.997163
H	-0.406660	-2.840154	2.490443
N	-0.899582	1.421275	-1.793581
H	-0.712230	0.501085	-2.165422

C	-1.577298	2.349453	-2.558149
O	-1.893289	3.445483	-2.121840
C	-1.860926	1.917252	-3.984345
H	-1.116404	2.370312	-4.646732
H	-2.841453	2.297260	-4.275954
H	-1.832038	0.832930	-4.120938
C	0.963149	-0.536458	3.236508
O	1.325984	-1.488493	3.881389
O	0.473472	0.574219	3.816032
H	0.332792	1.234807	3.111675

20HB

C	-1.398716	1.500065	1.109122
H	-1.545238	1.542987	2.190591
C	-1.325554	0.050526	0.582074
H	-1.692878	-0.747368	1.233204
N	0.153488	0.149310	0.499139
C	0.724393	-0.400699	-0.740515
H	1.103150	0.409644	-1.373688
C	-0.395262	-1.154698	-1.498340
S	-1.940828	-0.229297	-1.144477
C	0.082263	1.632957	0.682528
H	0.217905	2.181071	-0.257188
H	0.783483	2.017243	1.428358
H	-2.112550	2.160975	0.617227
H	-0.208222	-1.170930	-2.572190
H	-0.486293	-2.186677	-1.147629
C	1.905446	-1.346889	-0.449729
O	2.549522	-1.866288	-1.329784
O	2.129418	-1.549450	0.856724
H	1.456472	-0.992481	1.314572

21NHB

C	1.033079	-1.486573	-1.623225
H	1.158567	-2.561577	-1.475826
C	1.366930	-0.677401	-0.351288
H	1.972110	-1.154247	0.424787
N	-0.068373	-0.564395	-0.050730
C	-0.483048	0.765118	0.421076
H	-1.163640	1.212813	-0.313037
C	0.774028	1.642393	0.605151
S	1.995116	1.053728	-0.632891
C	-0.425310	-1.004190	-1.425277
H	-0.697310	-0.171853	-2.088327
H	-1.213670	-1.762315	-1.457971
H	1.532849	-1.179444	-2.542240
H	0.560999	2.698018	0.425622
H	1.162137	1.529246	1.619621
C	-1.247159	0.596085	1.735422
O	-0.788522	0.722256	2.848429
O	-2.532204	0.244616	1.504283
H	-2.936579	0.097723	2.376419

14 + H_2 → 19

C	1.014309	-0.441414	-1.437826
H	0.959278	-0.578470	-2.518463
C	-0.348577	-0.690135	-0.737358
H	-1.094638	-1.274929	-1.281342
N	-0.580357	0.759345	-0.704182
C	-1.129210	1.271339	0.542780
H	-0.368267	1.865277	1.064981
C	-1.521812	0.067349	1.485893
S	-0.279017	-1.254727	1.026374
C	-1.355038	0.445202	2.961123
H	-1.998423	1.299532	3.193031
H	-0.320742	0.720306	3.185228
H	-1.640645	-0.386803	3.611438
C	-2.945144	-0.453534	1.220162
H	-3.686731	0.293105	1.525930
H	-3.123839	-1.362462	1.799607
H	-3.109594	-0.682799	0.164160
N	2.175757	-1.134570	-0.960553
H	2.290178	-1.225232	0.039094
C	3.075768	-1.738941	-1.805656
O	2.976802	-1.686511	-3.023655
C	4.205169	-2.488240	-1.117108
H	4.102143	-3.554987	-1.336446
H	4.229806	-2.352493	-0.032463
H	5.155644	-2.158653	-1.543320
C	-2.313368	2.222466	0.379395
O	-2.644580	3.011291	1.241211
O	-2.976653	2.081177	-0.781793
H	-3.706805	2.723242	-0.749898
C	0.812014	1.054878	-1.047340
H	1.424712	1.334222	-0.170131
O	0.896300	2.034965	-2.044741
H	1.825560	2.281205	-2.148132

15 + H_2 → 17 (N1-C1-O1-H2 =180^0)

C	-0.914778	1.467861	-0.671955
H	-1.185116	2.498147	-0.415433
C	-0.996873	0.558352	0.578647
H	-1.616690	0.929279	1.397874
N	0.465172	0.738001	0.784144
C	1.184899	-0.494651	1.133803
H	1.771045	-0.839348	0.272911
C	0.153824	-1.613597	1.499208
S	-1.279439	-1.245471	0.340207
C	0.708297	-3.007621	1.195431
H	1.603535	-3.172378	1.801475
H	0.979211	-3.108162	0.140331
H	-0.025972	-3.780698	1.440076
C	-0.324851	-1.526034	2.957434
H	0.502247	-1.758793	3.634882
H	-1.127712	-2.245975	3.132213
H	-0.700495	-0.530224	3.210709
N	-1.539451	1.052017	-1.904178
H	-2.250491	0.336364	-1.889232
C	-1.064840	1.525133	-3.092224
O	-0.120927	2.314891	-3.141184
C	-1.760509	1.025854	-4.343698
H	-2.602871	0.359447	-4.142651
H	-1.030789	0.501827	-4.966934
H	-2.114702	1.888847	-4.913168
C	2.194597	-0.242299	2.273579
O	2.926957	-1.109953	2.693657
O	2.182061	1.004718	2.754643
H	1.523231	1.493697	2.209964
C	0.621274	1.297713	-0.575970
H	0.974162	0.536431	-1.288594
O	1.416715	2.434762	-0.587691
H	1.449279	2.711861	-1.518279

15 + H_2 → 18 (N1-C1-O1-H2 =60^0)

C	0.322974	1.055988	-1.413637
H	0.441158	1.055684	-2.498103

C	0.626787	-0.335362	-0.784678
H	1.164335	-1.047330	-1.415279
N	-0.833084	-0.599187	-0.661480
C	-1.239474	-1.108138	0.657188
H	-1.709086	-0.309056	1.245576
C	0.024917	-1.597523	1.435912
S	1.317726	-0.342330	0.921157
C	-0.188756	-1.526189	2.950614
H	-1.022309	-2.178411	3.225206
H	-0.424118	-0.507476	3.272340
H	0.705726	-1.860329	3.484197
C	0.464269	-3.009950	1.015767
H	-0.286664	-3.743717	1.326844
H	1.412190	-3.264651	1.495124
H	0.598398	-3.098053	-0.066101
N	0.996737	2.212585	-0.906761
H	1.026248	2.341690	0.094394
C	1.743413	3.039588	-1.718738
O	1.832420	2.870281	-2.925131
C	2.419088	4.199062	-1.007047
H	2.442529	4.093879	0.081065
H	1.890200	5.123857	-1.258031
H	3.439361	4.291418	-1.384416
C	-2.297930	-2.219772	0.506245
O	-2.866034	-2.714924	1.452110
O	-2.526982	-2.582009	-0.764178
H	-1.927636	-2.012600	-1.302746
C	-1.151262	0.819402	-1.015911
H	-1.466197	1.388374	-0.124562
O	-2.044208	0.993944	-2.071466
H	-2.884736	0.571255	-1.845472

Table S12. Energies (au) of component molecules for derivation of TA and COSNAR resonance energies of 3a and 6 in Table 3

Computational method		A 1-Azaadamantane	B 1-Azaadamantan-2-one	C N,N-Dimethylethylamine	D N,N-Dimethylacetamide	E 2-methylbutane	F 3-Methylbutanone
B3LYP/6-31G(d)	opt	-406.744846	-480.757440	-213.788638	-287.830189	-197.771176	-271.783203
B3LYP/6-31G(d)$_{298}$	freq	-406.504395	-480.535524	-213.631446	-287.691360	-197.602414	-271.633525
B3LYP/6-31G(d,p)	opt	-406.76524	-480.775131	-213.803286	-287.842522	-197.787926	-271.797239
B3LYP/6-31G(d,p)	freq	-406.525567	-480.553564	-213.646729	-287.704235	-197.619750	-271.648205
B3LYP/6-311+G(d,p)	opt	-406.848284	-480.886073	-213.85267	-287.918425	-197.829336	-271.866168
B3LYP/cc-pVTZ	opt	-406.880383	-480.9223619	-213.870673	-287.941195	-197.84733	-271.888092
M06-2X/6311++G(d,p)	opt	-406.670309	-480.688854	-213.733154	-287.779670	-197.709418	-271.728131
MP2/6-31G(d)opt	opt	-405.339229	-479.203523	-212.995424	-286.887867	-196.993365	-270.857617
MP2/6-31G(d.p)	opt	-405.460306	-479.307579	-213.084681	-286.959982	-197.091185	-270.938004
MP2/6-311+G(d,p)	opt	-405.6032467	-479.4929071	-213.165611	-287.080098	-197.160691	-271.049102
MP2/cc-pVTZ	opt	-405.86348	-479.7877373	-213.310352	-287.261648	-197.298068	-271.221299
G3MP2$_{elec}$		-406.225136	-480.167098	-213.518334	-287.486378	-197.508832	-271.450175
G3MP2$_{298}$		-405.994234	-479.953806	-213.367964	-287.353311	-197.348063	-271.306943
T1$_{298}$		-0.0120692	-0.0541485	-0.0169064	-0.0848662	-0.0573647	-0.0984405

TA 1-azaadamantan-2-one:2625.5×((B+C)-(A+D)) = W

COSNAR resonance energy *N,N*-dimethylacetamide: 2625.5×((D+E)-(C+F)) = X

G	H	I	J	K	L	M	N	O	P

		Azetidine	β-propiolactam	cyclobutanone	Cyclobutane	butane	butanone	1-aza-4-thiabicyclo-[3.2.0]heptane	1-aza-5-thiabicyclo-[3.2.0]heptan-2-one	5-thiabicyclo-[3.2.0]heptan-2-one	4-thiabicyclo-[3.2.0]heptane
B3LYP/											
6-31G(d)	opt	-173.237758	-247.285618	-231.228587	-157.213284	-158.458046	-232.470559	-648.852820	-722.892151	-706.839829	-632.826360
B3LYP/											
6-31G(d)$_{298}$	freq	-173.132598	-247.1992791	-231.1318863	-157.096829	-158.318786	-232.350813	-648.708066	-722.765889	-706.702732	-632.670062
B3LYP/											
6-31G(d,p)	opt	-173.249197	-247.294726	-231.237168	-157.224581	-158.471951	-232.481896	-648.865033	-722.901584	-706.851088	-632.840443
B3LYP/											
6-31G(d,p)	freq	-173.144349	-247.208561	-231.140660	-157.108573	-158.333185	-232.362492	-648.720787	-722.775834	-706.714530	-632.684647
B3LYP/											
6-311+G(d,p)	opt	-173.291526	-247.364133	-231.297936	-157.257312	-158.50548	-232.542969	-648.946464	-723.010207	-706.953186	-632.914865
B3LYP/											
cc-pVTZ	opt	-173.304603	-247.381777	-231.314736	-157.271491	-158.520121	-232.561127	-648.974423	-723.042955	-706.984896	-632.942829
M06-2X/											
6311++G(d,p)	opt	-173.201883	-247.253902	-231.188371	-157.168023	-158.404158	-232.423998	-648.800195	-722.843285	-706.787738	-632.768999
MP2/											
6-31G(d)	opt	-172.629475	-246.527751	-230.483526	-156.617991	-157.826036	-231.690795	-647.434747	-721.325219	-705.287826	-631.422684
MP2/											
6-31G(d.p)	opt	-172.687595	-246.568823	-230.53089	-156.682787	-157.907454	-231.754761	-647.506982	-721.380374	-705.351185	-631.503305
MP2/											
6-311+G(d,p)	opt	-172.754555	-246.675885	-230.627054	-156.737119	-157.962661	-231.851322	-647.631713	-721.545989	-705.507203	-631.617930
MP2/cc-pVTZ	opt	-172.866128	-246.824735	-230.767623	-156.842538	-158.07392	-231.99781	-647.840560	-721.790994	-705.744252	-631.819892
G3MP2$_{elec}$		-173.021121	-246.996021	-230.943622	-156.999762	-158.245350	-232.187510	-648.100518	-722.067434	-706.025261	-632.082598
G3MP2$_{298}$		-172.920155	-246.912787	-230.850553	-156.888615	-158.112758	-232.072792	-647.961205	-721.945415	-705.893087	-631.932686

$T1_{298}$	0.040633	-0.034388	-0.031770	0.011318	-0.047741	-0.089304	0.050866	-0.016103	-0.024041	0.018380

β-propiolactam (3a):

E_{TA} (kJmol^{-1}) = 2625.5×((H+C)-(G+D))=Y1

$E_{corr=}$(kJmol^{-1}) = 2625.5×((I+K)-(J+L))=Z1

RE_{TA}(kJmol^{-1}) = –(W–(Y1–Z1))

RE_{COSNAR} (kJmol^{-1}) = 2625.5×((H+J)-(G+I))

1-Aza-5-thiabicyclo[3.2.0]heptan-2-one (penam)(6):

E_{TA} (kJmol^{-1}) = 2625.5×((N+C)-(M+D))=Y2

$E_{corr(}$(kJmol^{-1}) = 2625.5×((O+K)-(P+L))=Z2

RE_{TA}(kJmol^{-1}) = –(W–(Y2–Z2))

RE_{COSNAR}(kJmol^{-1}) = 2625.5×((N+P)-(M+O))

Amidicities (%):

TA= –(100×RE_{TA}/W)
COSNAR = 100× RE_{COSNAR}/X

Table S13 B3LYP/6-31G(d) structures for TA and COSNAR data in Table 4 and Table 6

The "penamine" corresponds to the 1-aza-4-thiabicyclo[3.2.0]heptane;
The "penam" corresponds to the 1-aza-4-thiabicyclo[3.2.0]heptan-7-one;
The "penone" corresponds to the 2-thiabicyclo[3.2.0]heptan-6-one;
The "penane" corresponds to the 2-thiabicyclo[3.2.0]heptane.

Penamine and lactam structures are common to both the TA and COSNAR methodologies. COSNAR uses, additionally, the corresponding penones and penanes.
ΔE_{corr} from Equation 10 utilises B3LYP/6-31G(d) structures of butanone and butane as well as the corresponding penanes and penones.

Butanone

H	2.680577	-0.271896	-0.029782
C	1.899187	0.489741	0.007231
H	2.022594	1.094592	0.914606
H	2.007891	1.171044	-0.845773
C	0.530579	-0.173607	-0.004012
O	0.408829	-1.383960	-0.004038
C	-0.677806	0.757874	-0.013086
H	-0.584747	1.441535	0.844009
H	-0.595779	1.404060	-0.900082
C	-2.016764	0.024036	0.009729
H	-2.105805	-0.598500	0.905071
H	-2.113497	-0.637926	-0.855864
H	-2.849112	0.735405	-0.002105

Butane

C	-0.516705	-0.000199	-0.567532
H	-1.169024	-0.878531	-0.459791
H	-1.169133	0.878010	-0.459474
C	0.118356	0.000142	-1.961641
H	0.751213	-0.884118	-2.107836
H	0.750339	0.884982	-2.107930
H	-0.642066	-0.000268	-2.750989
C	0.516705	-0.000206	0.567532
H	1.169141	0.877997	0.459474
H	1.169015	-0.878544	0.459790
C	-0.118356	0.000140	1.961641
H	-0.750351	0.884972	2.107923
H	0.642066	-0.000251	2.750988
H	-0.751198	-0.884127	2.107846

Penam 6_{ax}

Penamine

C	-1.045813	0.658641	0.267106
H	-1.700505	1.126333	1.007390
N	0.371672	0.547984	0.632758
C	0.726049	-0.782096	1.102553
H	0.452683	-0.864435	2.160880
H	1.809431	-0.926549	1.019140
C	-0.054582	-1.837521	0.283242
S	-1.703905	-1.082921	-0.027820
C	0.784994	0.965206	-0.735116
H	1.065820	0.129030	-1.391268
H	1.590046	1.707589	-0.740666
H	0.443995	-2.066759	-0.663414
H	-0.187336	-2.768891	0.839856
C	-0.656326	1.470760	-0.988584
H	-0.767828	2.548766	-0.839968
H	-1.128394	1.174864	-1.926088

Lactam

C	-0.622218	1.461591	-1.148324
H	-0.846277	2.532776	-1.155051
C	-1.030116	0.697271	0.141363
H	-1.645611	1.237966	0.862882
C	0.818948	1.090607	-0.743529
O	1.913092	1.129360	-1.246041
N	0.390871	0.582967	0.496799
C	0.812548	-0.683555	1.073606
H	0.611187	-0.687090	2.149735
H	1.887687	-0.804433	0.912055
C	-0.005603	-1.779501	0.352934
S	-1.671179	-1.046858	0.006718
H	-0.946837	1.006165	-2.086430
H	0.473929	-2.066159	-0.586665
H	-0.140419	-2.671109	0.969948

Penone

C	-0.637652	1.262284	-1.274515
H	-0.871833	2.330358	-1.372220
C	-1.109543	0.641555	0.077038
H	-1.820322	1.241300	0.646954
C	0.808817	1.026651	-0.816008
O	1.881914	1.075748	-1.359521
C	0.769141	-0.799451	1.069110
H	0.510933	-0.920159	2.126830
H	1.849514	-0.953746	0.961514
C	-0.021543	-1.805179	0.220807
S	-1.716906	-1.095017	0.027049
C	0.367356	0.602427	0.602372
H	0.602127	1.373792	1.345742
H	-0.112809	-2.782966	0.700784
H	0.439509	-1.948765	-0.761949
H	-0.938704	0.751168	-2.193986

Penane

C	-0.979572	1.444027	-0.652584
H	-0.865236	2.531815	-0.722766
C	-0.548025	0.910976	0.741888
H	-0.474213	1.653190	1.540573
C	1.038621	-1.072515	0.508951
H	1.546811	-1.105811	1.480183
H	1.680181	-1.583980	-0.220953
C	-0.323946	-1.770468	0.624921
S	-1.456292	-0.544700	1.416030
C	0.784583	0.383151	0.114761
C	0.203771	0.673524	-1.300916
H	0.848597	1.246287	-1.974464
H	1.644427	1.019216	0.350842
H	-0.112186	-0.235644	-1.823705
H	-0.286402	-2.662740	1.255983
H	-0.714189	-2.063903	-0.354822
H	-1.986932	1.177577	-0.983922

Penam 6_{eq}

Penamine

C	-0.885603	-0.035774	-0.727576
H	-1.418937	0.618798	-1.424520
N	0.534863	0.275226	-0.528779
C	0.827214	1.018603	0.700360
H	1.397173	1.932064	0.484660
C	-0.504288	1.390863	1.395341
S	-1.708117	0.076037	0.946927
C	0.890374	-1.164643	-0.615829
H	1.051870	-1.631064	0.366624
H	1.753215	-1.372157	-1.258468
C	-0.513005	-1.458222	-1.198764
H	-0.522665	-1.551248	-2.287992
H	-1.069988	-2.284557	-0.754322
H	1.439391	0.395545	1.365491
H	-0.399564	1.426405	2.482843
H	-0.871934	2.364121	1.054006

Lactam

C	-0.335619	1.048711	-1.718651
H	-0.299990	2.097098	-2.027422
C	-0.792914	0.808200	-0.255694
H	-1.221383	1.655156	0.285523
C	1.010690	0.465574	-1.239053
O	2.029913	0.070396	-1.744892
N	0.593969	0.480932	0.099182
C	0.823034	-0.580070	1.074567
H	1.304763	-0.194599	1.979862
C	-0.565266	-1.182880	1.432142
S	-1.744496	-0.742534	0.080386
H	-0.836518	0.448894	-2.480635
H	-0.525605	-2.271979	1.511732
H	1.489967	-1.320551	0.620904
H	-0.930545	-0.782346	2.382050

Penone

C	-0.478018	0.777188	-1.725878
H	-0.779460	1.669112	-2.286049
C	-0.945738	0.698810	-0.239094
H	-1.470455	1.594653	0.098071
C	0.970495	0.814289	-1.210684
O	2.039611	0.982305	-1.736699
C	0.806059	-0.812701	0.828397
H	1.628922	-0.798265	1.551633
C	-0.501451	-1.291472	1.471046
S	-1.845072	-0.811714	0.300312
C	0.537564	0.597311	0.253064
H	0.857941	1.385182	0.943298
H	-0.710831	-0.110089	-2.324247
H	1.088218	-1.503250	0.025806
H	-0.527732	-2.376296	1.608393
H	-0.670053	-0.815064	2.442631

Penane

C	1.207535	0.900755	-0.992795
H	1.677429	1.214804	-1.929913
C	0.459004	-0.462682	-1.020093
H	0.216916	-0.788513	-2.034878
C	-0.645748	-0.233376	1.204684
C	-0.237611	-1.710898	1.230574
S	1.093213	-1.892262	-0.043659
C	-0.735668	0.194758	-0.268828
C	-0.135811	1.588523	-0.616367
H	-0.624364	2.045159	-1.482762
H	-1.727310	-0.026283	-0.678550
H	-0.110458	2.325316	0.193820
H	0.159612	-2.020404	2.201324
H	1.953983	0.947106	-0.194990
H	-1.593710	-0.072768	1.733870
H	-1.078518	-2.365894	0.978259
H	0.121506	0.356658	1.720302

Penam-3-carboxylic acid 23_{ax} HB

Penamine

C	0.832534	-1.290531	-1.621543
H	1.142278	-2.339168	-1.642188
C	1.210476	-0.571856	-0.303334
H	1.917494	-1.086890	0.351800
N	-0.211107	-0.634019	0.142658
C	-0.701706	0.653785	0.635449
H	-1.784753	0.700721	0.459253
C	0.007308	1.802497	-0.101657
S	1.726773	1.211902	-0.374100
C	-0.645908	-1.082161	-1.215936
H	-1.154048	-0.295214	-1.786813
H	-1.283899	-1.970474	-1.188238
C	-0.511203	0.743247	2.166954
O	-0.542373	1.785556	2.774256
O	-0.363256	-0.452617	2.758028
H	-0.341471	-1.107292	2.019763
H	1.155869	-0.796307	-2.538421
H	-0.481214	2.027950	-1.053968
H	0.028206	2.700873	0.518037

Lactam

C	-1.382701	-0.855699	-1.681666
H	-2.390689	-1.281324	-1.695356
C	-0.505355	-1.237955	-0.456776
H	-0.906474	-2.006417	0.205853
C	-1.290271	0.580173	-1.142923
O	-1.557457	1.688443	-1.520250
N	-0.650388	0.148570	0.053217
C	0.566722	0.767777	0.574608
H	0.478531	1.850550	0.421700
C	1.755702	0.202909	-0.226608
S	1.307952	-1.533121	-0.683833
C	0.714930	0.531354	2.091321
O	1.775727	0.590665	2.659804
O	-0.443195	0.301305	2.736182
H	-1.152368	0.260330	2.062731
H	-0.911083	-0.989924	-2.657536
H	1.932695	0.794321	-1.128170
H	2.657723	0.188042	0.387700

Penone

C	-0.539748	1.373576	-1.826013
H	-0.625426	2.456103	-1.982847
C	-1.002931	0.924246	-0.407011
H	-1.600421	1.646871	0.149600
C	0.884908	0.955975	-1.434171
O	1.906811	0.776152	-2.039963
C	0.753008	-0.682969	0.607912
H	1.788026	-0.965242	0.392296
C	-0.218049	-1.630021	-0.125204
S	-1.825289	-0.722230	-0.294267
C	0.485230	0.725121	0.043571

H	0.871851	1.516034	0.696654
C	0.633120	-0.694564	2.140640
O	1.602895	-0.654993	2.857210
O	-0.613965	-0.714465	2.660202
H	-1.289790	-0.724344	1.946626
H	-0.973111	0.858273	-2.688423
H	0.169114	-1.884083	-1.115717
H	-0.406234	-2.559439	0.418904

Penane

C	-1.266517	1.519875	-1.076359
H	-1.236433	2.598697	-1.259339
C	-0.734148	1.147519	0.334546
H	-0.589894	1.976909	1.030589
C	0.750771	-0.943587	0.125897
H	1.237836	-1.505685	-0.677239
C	-0.651835	-1.525604	0.399710
S	-1.615336	-0.192041	1.244493
C	0.546507	0.522034	-0.315118
C	-0.082711	0.747187	-1.722621
H	0.537439	1.318742	-2.418448
H	1.452580	1.113202	-0.151908
H	-0.380785	-0.182794	-2.218246
C	1.712947	-1.039379	1.319416
O	2.863246	-1.384151	1.190302
O	1.228560	-0.682510	2.529208
H	0.278111	-0.433862	2.460320
H	-2.269895	1.155784	-1.310838
H	-0.633489	-2.404585	1.050071
H	-1.146954	-1.805750	-0.534435

Penam-3-carboxylic acid 23_{eq} HB

Penamine

C	-1.399507	1.503349	1.105866
H	-1.552423	1.549378	2.187047
C	-1.328049	0.052445	0.580816
H	-1.694646	-0.742831	1.236206
N	0.151478	0.148310	0.499616
C	0.722093	-0.399860	-0.740724
H	1.094043	0.412764	-1.375636
C	-0.396730	-1.159074	-1.495020
S	-1.943010	-0.232513	-1.144574
C	0.084066	1.631451	0.686293
H	0.227611	2.181211	-0.251846
H	0.783759	2.009892	1.437320
H	-2.108753	2.165965	0.607979
H	-0.208179	-1.179849	-2.569344
H	-0.485905	-2.190574	-1.140051
C	1.908382	-1.341567	-0.454838
O	2.557058	-1.850414	-1.337415
O	2.132048	-1.555282	0.851181
H	1.456665	-1.002801	1.317125

Lactam

C	-1.207893	-1.466669	-1.501959
H	-2.249759	-1.381258	-1.824291
C	-0.956851	-1.138726	-0.007183
H	-1.827774	-1.059041	0.646383
C	-0.355239	-0.216573	-1.780872
O	0.195433	0.288600	-2.719731
N	-0.368543	0.162388	-0.410840
C	0.819107	0.618505	0.321904
H	1.644830	0.712433	-0.392903
C	1.140242	-0.459774	1.395413
S	0.423371	-2.050377	0.806983
C	0.636260	1.995985	0.984059
O	1.463380	2.452133	1.734140
O	-0.498106	2.643607	0.667327
H	-1.006862	2.063539	0.064597
H	-0.776621	-2.398962	-1.871003
H	2.216621	-0.581428	1.527222
H	0.708403	-0.184384	2.360755

Penone

C	-1.437359	1.377279	-1.593407
H	-1.335171	2.461966	-1.727594
C	-1.361641	0.955484	-0.096210
H	-1.598922	1.724028	0.641349
C	-0.090611	0.661753	-1.787615
O	0.506207	0.226155	-2.734142
C	0.492665	-0.821168	0.331538
H	0.727392	-1.489353	-0.506158
C	-0.742938	-1.327451	1.100999
S	-2.224188	-0.623942	0.269251
C	0.143106	0.568478	-0.261682
H	0.822586	1.362525	0.069553
C	1.726986	-0.775855	1.218025
O	1.758493	-0.970326	2.413072
O	2.833023	-0.473636	0.496687
H	3.576778	-0.455555	1.128555
H	-2.278255	1.019416	-2.192498
H	-0.821699	-2.417637	1.087446
H	-0.696452	-1.002161	2.142830

Penane

C	-1.453106	1.424197	-0.980721
H	-1.947111	2.374758	-1.202578
C	-1.238638	1.093889	0.525216
H	-1.302392	1.978753	1.163098
C	0.244764	-0.881028	0.174353
H	-0.197166	-1.220163	-0.768425
C	-0.622048	-1.362842	1.345306
S	-2.137007	-0.309643	1.312561
C	0.222165	0.669562	0.205627
C	0.090252	1.372567	-1.173553
H	0.544124	2.368006	-1.170172
H	0.989969	1.045990	0.889980
H	0.472399	0.819890	-2.037305
C	1.667155	-1.398738	0.250927
O	2.272918	-1.670191	1.264208
O	2.228837	-1.487414	-0.981373
H	3.148620	-1.782990	-0.839278
H	-1.979051	0.623890	-1.508643
H	-0.088606	-1.247815	2.292125
H	-0.916078	-2.410678	1.238647

Penam-3-carboxylic acid 24_{ax} NHB

Penamine

C	0.882085	-1.647621	1.529188
H	1.085691	-1.544963	2.599020
C	1.198566	-0.352967	0.747158
H	1.891563	0.372973	1.174878
N	-0.221110	0.012376	0.794511
C	-0.706509	0.567955	-0.449134
H	-1.795155	0.454456	-0.508731

C	-0.032743	-0.188968	-1.635234
S	1.672884	-0.570622	-1.068564
C	-0.599444	-1.377332	1.166078
H	-0.948844	-1.987246	0.320826
H	-1.337417	-1.427976	1.973290
C	-0.388363	2.060636	-0.513900
O	0.344097	2.668835	0.227925
O	-1.034324	2.642651	-1.557667
H	-0.760679	3.579225	-1.555761
H	1.326223	-2.570379	1.154334
H	-0.581656	-1.108773	-1.855893
H	0.005134	0.417738	-2.542324

Lactam

C	-1.935166	-0.697595	-1.444021
H	-3.005165	-0.847236	-1.272793
C	-1.004426	-1.100497	-0.266462
H	-1.449458	-1.642800	0.567688
C	-1.421995	0.732567	-1.180509
O	-1.468465	1.804602	-1.727065
N	-0.756616	0.323767	-0.010204
C	0.589815	0.693570	0.358451
H	0.756978	1.743658	0.098364
C	1.528954	-0.222760	-0.480386
S	0.661579	-1.848705	-0.641312
C	0.806691	0.512766	1.858687
O	0.023251	0.018227	2.631739
O	2.029103	0.971708	2.219595
H	2.113824	0.807968	3.177925
H	-1.653362	-1.092619	-2.422094
H	2.497428	-0.377920	-0.001040
H	1.687031	0.221299	-1.466563

Penone

C	-0.457849	1.378519	-2.003600
H	-0.455472	2.449866	-2.241600
C	-0.990529	1.060984	-0.571183
H	-1.517411	1.874761	-0.072158
C	0.919746	0.880933	-1.543027
O	1.946578	0.600663	-2.105469
C	0.579963	-0.624338	0.563176
H	1.583856	-1.037671	0.389570
C	-0.464883	-1.525944	-0.125640
S	-1.969282	-0.482545	-0.361727
C	0.464853	0.760762	-0.074480
H	0.889310	1.536193	0.571060
C	0.397125	-0.538742	2.075377
O	0.433010	0.476968	2.732587
O	0.229273	-1.762023	2.631235
H	0.135554	-1.614268	3.591150
H	-0.906708	0.833728	-2.839633
H	-0.086502	-1.872174	-1.092179
H	-0.730632	-2.395672	0.476540

Penane

C	-1.393536	1.566493	-1.080142
H	-1.292088	2.656799	-1.122402
C	-1.032468	1.015510	0.327294
H	-1.042495	1.736017	1.148731
C	0.667846	-0.890207	0.156376
H	1.332371	-1.331697	-0.602611
C	-0.664150	-1.655788	0.186717
S	-1.912152	-0.497925	0.898783
C	0.357520	0.564686	-0.225143
C	-0.158080	0.831682	-1.669756
H	0.504390	1.419852	-2.311826
H	1.168470	1.237882	0.059271
H	-0.424386	-0.087052	-2.202216
C	1.412068	-1.041453	1.481667
O	1.238054	-1.922706	2.292502
O	2.369114	-0.092587	1.642861
H	2.808392	-0.299081	2.489450
H	-2.374222	1.290290	-1.476163
H	-0.603997	-2.537681	0.826524
H	-0.960652	-1.963036	-0.819916

Penam-3-carboxylic acid 24_{eq} NHB

Penamine

C	1.033878	-1.485525	-1.624915
H	1.164034	-2.560971	-1.479362
C	1.369590	-0.675744	-0.353347
H	1.974601	-1.154971	0.422057
N	-0.065273	-0.565175	-0.049291
C	-0.481656	0.763994	0.421420
H	-1.160272	1.210827	-0.315394
C	0.774998	1.642427	0.606334
S	1.995447	1.055936	-0.634240
C	-0.425356	-1.007711	-1.421752
H	-0.702695	-0.175884	-2.084101
H	-1.212671	-1.767663	-1.449491
H	1.529199	-1.175213	-2.546208
H	0.559579	2.698832	0.428937
H	1.164848	1.529393	1.620719
C	-1.247877	0.594998	1.734585
O	-0.790077	0.710702	2.849065
O	-2.536832	0.255582	1.500088
H	-2.943462	0.106166	2.374897

Lactam

C	-2.028784	-0.995275	-1.288427
H	-3.058282	-0.631119	-1.344101
C	-1.366403	-0.881271	0.109841
H	-2.007123	-0.633419	0.958333
C	-0.956759	0.026585	-1.723122
O	-0.528740	0.473891	-2.754942
N	-0.552845	0.230862	-0.393982
C	0.817820	0.348358	0.064068
H	1.483076	0.328996	-0.804570
C	1.085898	-0.878951	1.000759
S	-0.135458	-2.187653	0.563464
C	1.062090	1.634923	0.849915
O	0.232912	2.249278	1.475383
O	2.372472	1.973485	0.801631
H	2.473046	2.773545	1.351559
H	-1.945185	-1.966272	-1.779972
H	2.095780	-1.270871	0.864933
H	0.956485	-0.595091	2.049230

Penone

Penam-3-carboxylic acid 24_{ax} NHB Penone

Penane

Penam-3-carboxylic acid 24_{ax} NHB Penane

2,2-Dimethylpenam 25_{ax}

Penamine

C	-0.764968	2.293835	-1.156360
H	-0.973045	3.357717	-1.010270
C	-1.158968	1.436830	0.068468
H	-1.864632	1.863839	0.787629
N	0.240647	1.396198	0.489015
C	0.651567	0.107798	1.009320
H	0.438150	0.085783	2.085962
H	1.735621	-0.006719	0.889408
C	-0.109154	-1.084616	0.330032
S	-1.706513	-0.324611	-0.277534
C	0.678459	-1.697537	-0.841810
H	1.619650	-2.131132	-0.476654
H	0.918329	-0.959046	-1.610417
H	0.106045	-2.499434	-1.320565
C	-0.416669	-2.179720	1.363854
H	0.519553	-2.600620	1.755605
H	-0.986547	-3.001891	0.917805
H	-0.995441	-1.782607	2.203159
C	0.699152	1.901763	-0.831658
H	1.104842	1.134889	-1.502884
H	1.424231	2.719494	-0.752248
H	-1.160307	1.969788	-2.119855

Lactam

C	-0.764968	2.293835	-1.156360
H	-0.973045	3.357717	-1.010270
C	-1.158968	1.436830	0.068468
H	-1.864632	1.863839	0.787629
N	0.240647	1.396198	0.489015
C	0.651567	0.107798	1.009320
H	0.438150	0.085783	2.085962
H	1.735621	-0.006719	0.889408
C	-0.109154	-1.084616	0.330032
S	-1.706513	-0.324611	-0.277534
C	0.678459	-1.697537	-0.841810
H	1.619650	-2.131132	-0.476654
H	0.918329	-0.959046	-1.610417
H	0.106045	-2.499434	-1.320565
C	-0.416669	-2.179720	1.363854
H	0.519553	-2.600620	1.755605
H	-0.986547	-3.001891	0.917805
H	-0.995441	-1.782607	2.203159
C	0.699152	1.901763	-0.831658
H	1.104842	1.134889	-1.502884
H	1.424231	2.719494	-0.752248
H	-1.160307	1.969788	-2.119855

Penone

C	-0.672251	2.089991	-1.354050
H	-0.919228	3.154106	-1.461895
C	-1.185352	1.456100	-0.023922
H	-1.915124	2.054061	0.524073
C	0.761164	1.877329	-0.840800
O	1.854605	1.987404	-1.332840
C	0.651658	0.041348	1.081736
H	0.382828	-0.012751	2.143063
H	1.734638	-0.120263	1.007432
C	-0.115190	-1.058865	0.306863
S	-1.780606	-0.278487	-0.087219
C	0.608464	-1.478035	-0.984228
H	1.563532	-1.961203	-0.738447
H	0.826493	-0.630703	-1.639013
H	0.002650	-2.192027	-1.551231
C	-0.359929	-2.295700	1.182613
H	0.598243	-2.758790	1.450701
H	-0.951863	-3.048283	0.650036
H	-0.889093	-2.034040	2.103795
C	0.268959	1.425311	0.551961
H	0.466629	2.208546	1.294943
H	-0.931226	1.574951	-2.283571

Penane

C	2.050367	0.873768	-0.927899
H	3.119905	1.056640	-1.076552
C	1.687115	0.428782	0.519810
H	2.531939	0.394566	1.212329
C	-0.286382	-1.172998	0.346063
H	-0.327369	-1.769964	1.264893
H	-0.812238	-1.744812	-0.431105
C	-1.019829	0.168192	0.613231
S	0.297369	1.257593	1.380204
C	-1.587397	0.808822	-0.666293
H	-2.326772	0.139449	-1.127126
H	-0.811065	1.017859	-1.405988
H	-2.085945	1.755646	-0.433874
C	-2.150646	-0.009865	1.636524
H	-2.933496	-0.660374	1.225028
H	-2.617182	0.950324	1.883696
H	-1.780478	-0.458486	2.563369
C	1.185657	-0.949322	-0.026703
C	1.549428	-0.494715	-1.472846
H	2.325968	-1.104261	-1.945073
H	1.789295	-1.798248	0.310710
H	0.701076	-0.438856	-2.161614
H	1.500680	1.750259	-1.280785

2,2-Dimethylpenam 25_{eq}

Penamine

C	-0.294698	2.168511	-1.695321
H	-0.478508	3.236825	-1.553078
C	-0.781014	1.324544	-0.497362
H	-1.489279	1.793966	0.193034
N	0.600804	1.220209	-0.000371
C	0.977309	-0.124100	0.442628
H	1.456642	-0.095217	1.431464
C	-0.280501	-1.034431	0.514952
S	-1.357695	-0.402962	-0.874976
C	0.075227	-2.504320	0.264902
H	0.774351	-2.857370	1.034047
H	0.542013	-2.641565	-0.715681
H	-0.815927	-3.139016	0.315043
C	-1.001984	-0.881827	1.864796
H	-0.361433	-1.246645	2.679460
H	-1.931448	-1.459717	1.874134
H	-1.248518	0.163405	2.077687
C	1.132805	1.725825	-1.292381
H	1.536108	0.929964	-1.935670
H	1.886851	2.513622	-1.184441
H	-0.645797	1.865318	-2.682803
H	1.704693	-0.555017	-0.260064

Lactam

C	-0.283744	2.102418	-1.954517
H	-0.409561	3.188408	-1.983657
C	-0.723559	1.422580	-0.631747

H	-1.278297	2.035217	0.083013
C	1.127917	1.614260	-1.566161
O	2.202561	1.515827	-2.102481
N	0.693355	1.210572	-0.297362
C	1.061541	-0.037686	0.362945
H	1.525686	0.147799	1.338765
C	-0.234856	-0.890559	0.559609
S	-1.432861	-0.275176	-0.748691
C	0.039247	-2.380776	0.328369
H	0.776168	-2.741808	1.057013
H	0.429899	-2.562112	-0.677489
H	-0.871250	-2.975851	0.457140
C	-0.826706	-0.659879	1.959898
H	-0.131137	-1.022411	2.728612
H	-1.774420	-1.193882	2.076798
H	-1.012289	0.402654	2.150491
H	-0.670492	1.654914	-2.872059
H	1.792798	-0.554512	-0.268491

Penone

C	-0.274947	1.997724	-1.934551
H	-0.693957	2.991665	-2.131100
C	-0.904534	1.244799	-0.722313
H	-1.743063	1.767861	-0.258381
C	1.049838	2.042407	-1.155520
O	2.150428	2.460869	-1.403191
C	0.997499	-0.091112	0.367829
H	1.569206	-0.109207	1.303543
H	1.680114	-0.404266	-0.430099
C	-0.189841	-1.078382	0.438668
S	-1.296674	-0.529616	-0.968962
C	0.246259	-2.526690	0.190067
H	0.920626	-2.857777	0.989907
H	0.768717	-2.628363	-0.766382
H	-0.615825	-3.202916	0.185528
C	-0.934375	-0.966349	1.778227
H	-0.278503	-1.277461	2.602811
H	-1.820414	-1.608273	1.784599
H	-1.261674	0.059490	1.978022
C	0.448379	1.319933	0.067311
H	0.414702	1.954173	0.960240
H	-0.231962	1.441490	-2.876254

Penane

C	1.916686	1.062692	-1.378872
H	2.904218	1.514818	-1.512131
C	1.510105	0.712201	0.082269
H	2.366066	0.678993	0.761066
C	-0.503204	-0.650912	-0.472548
H	-0.933025	-1.660976	-0.510962
C	-1.046950	0.123212	0.747078
S	0.109799	1.600680	0.877379
C	-2.477724	0.625207	0.523263
H	-3.163556	-0.225137	0.414435
H	-2.545745	1.242407	-0.378002
H	-2.826354	1.222834	1.373048
C	-0.970361	-0.713803	2.033826
H	-1.629712	-1.589980	1.959296
H	-1.285230	-0.124969	2.901421
H	0.046891	-1.068818	2.225867
C	1.030574	-0.688548	-0.403200
C	1.782109	-0.443327	-1.743249
H	2.749698	-0.953963	-1.774862
H	1.380109	-1.538442	0.191822
H	1.233682	-0.687126	-2.659644
H	1.173270	1.693958	-1.872431
H	-0.821348	-0.131001	-1.384869

2,2-Dimethylpenam-3-carboxylic acid 26_{ax} HB

Penamine

C	0.761125	-1.925492	-1.612495
H	1.172446	-2.911294	-1.844601
C	1.263071	-1.311175	-0.278600
H	1.954835	-1.946508	0.282302
N	-0.127004	-1.323866	0.271278
C	-0.608349	-0.009102	0.721196
H	-1.654939	0.093179	0.407342
C	0.217009	1.150867	0.047862
S	1.911638	0.397392	-0.196071
C	-0.405713	1.530459	-1.309474
H	-1.401548	1.967870	-1.158424
H	-0.507128	0.675773	-1.983668
H	0.217119	2.274823	-1.814767
C	0.388942	2.425304	0.888129
H	-0.584662	2.876341	1.099496
H	0.990929	3.149645	0.327920
H	0.876753	2.228199	1.842939
C	-0.658319	-1.923676	-0.990694
H	-1.399970	-1.298373	-1.497980
H	-1.095209	-2.912649	-0.818536
C	-0.666956	0.011039	2.272765
O	-1.043347	0.967771	2.908507
O	-0.330784	-1.154956	2.839589
H	-0.153155	-1.759838	2.074423
H	0.883216	-1.271732	-2.478439

Lactam

C	-2.154025	-1.018465	-1.510553
H	-3.167340	-1.429291	-1.470057
C	-1.226606	-1.401082	-0.322239
H	-1.623268	-2.146976	0.370134
C	-2.017572	0.423853	-0.993237
O	-2.300242	1.530067	-1.368210
N	-1.322295	-0.005402	0.167302
C	-0.107719	0.601594	0.707607
H	-0.162885	1.676709	0.499816
C	1.115155	0.004211	-0.089370
S	0.560218	-1.726032	-0.601617
C	1.367303	0.865077	-1.340992
H	1.757282	1.847030	-1.043264
H	0.459093	1.028065	-1.928005
H	2.107947	0.387639	-1.989211
C	2.422830	-0.144015	0.699834
H	2.770343	0.832900	1.047383
H	3.192057	-0.569768	0.045872
H	2.311445	-0.790169	1.570887
C	-0.070274	0.482593	2.248903
O	0.871935	0.833942	2.914219
O	-1.202939	0.015085	2.806985
H	-1.848242	-0.124766	2.083674
H	-1.732202	-1.172800	-2.505859

Penone

C	0.746559	-2.184949	-1.749432
H	0.904017	-3.268468	-1.826747
C	1.184700	-1.583548	-0.377212

H	1.812591	-2.223950	0.242617
C	-0.702827	-1.835505	-1.377239
O	-1.747749	-1.821582	-1.974799
C	-0.662546	-0.056998	0.596596
H	-1.695590	0.198889	0.334233
C	0.283995	1.006108	-0.079611
S	1.898698	0.102268	-0.388970
C	-0.332590	1.491501	-1.404159
H	-1.247141	2.066375	-1.206138
H	-0.594236	0.667607	-2.071587
H	0.371581	2.141755	-1.932097
C	0.600765	2.225442	0.800236
H	-0.315653	2.777040	1.036445
H	1.274850	2.903876	0.266334
H	1.088128	1.938047	1.735680
C	-0.305534	-1.448880	0.064030
H	-0.610081	-2.232617	0.766787
C	-0.567038	-0.053374	2.115121
O	0.143799	-0.772212	2.781910
O	-1.401680	0.861717	2.667866
H	-1.263277	0.808681	3.632928
H	1.136259	-1.707223	-2.652792

Penane

C	-1.138872	2.205456	-1.145487
H	-1.273817	3.281096	-1.298462
C	-0.656983	1.830692	0.287648
H	-0.535708	2.676961	0.967349
C	0.845808	-0.239946	0.044709
H	1.241012	-0.792864	-0.815253
C	-0.543244	-0.883989	0.429093
S	-1.518929	0.507297	1.204673
C	-1.255243	-1.420431	-0.827109
H	-0.667767	-2.228215	-1.284811
H	-1.412246	-0.644771	-1.579717
H	-2.236883	-1.824399	-0.559793
C	-0.447208	-2.016271	1.464710
H	0.142521	-2.851263	1.070469
H	-1.448776	-2.391879	1.699822
H	0.008714	-1.674541	2.397987
C	0.667119	1.251325	-0.305469
C	0.181062	1.630882	-1.736121
H	0.816305	2.372981	-2.228867
H	1.551944	1.809947	0.007562
H	0.057793	0.788991	-2.424032
C	1.864170	-0.386201	1.164839
O	2.058711	0.402343	2.062865
O	2.574122	-1.539819	1.048994
H	3.179924	-1.559715	1.814417
H	-2.053529	1.696332	-1.460015

2,2-Dimethylpenam-3-carboxylic acid 26_{eq} HB

Penamine

C	0.970977	-2.090238	-1.783078
H	1.302596	-3.114723	-1.594464
C	1.226615	-1.148364	-0.585836
H	1.885638	-1.520334	0.203591
N	-0.220121	-1.184524	-0.234294
C	-0.800278	0.139717	0.036046
H	-1.390255	0.480082	-0.823330
C	0.357148	1.170858	0.263835
S	1.635023	0.603822	-0.978767
C	-0.095990	2.595612	-0.070007
H	-0.927890	2.871690	0.585634
H	-0.431824	2.673815	-1.109255
H	0.720614	3.308701	0.084000
C	0.931816	1.108517	1.689734
H	0.179394	1.439187	2.414502
H	1.799853	1.767960	1.770686
H	1.248490	0.097907	1.967274
C	-0.538094	-1.864008	-1.529286
H	-1.012190	-1.192117	-2.256052
H	-1.158959	-2.757241	-1.411580
C	-1.757889	0.083359	1.243426
O	-2.457699	1.013955	1.571493
O	-1.726133	-1.082934	1.905198
H	-1.095153	-1.645468	1.388350
H	1.354311	-1.755228	-2.747818

Lactam

C	-2.198511	-1.114720	-1.738621
H	-3.143667	-1.620909	-1.522352
C	-1.080589	-1.338588	-0.688647
H	-1.259808	-2.109254	0.063615
C	-2.144365	0.355421	-1.291038
O	-2.559167	1.412510	-1.679981
N	-1.287532	0.050928	-0.197387
C	-0.082425	0.834797	0.113594
H	0.026575	1.623738	-0.638623
C	1.152031	-0.137586	0.030004
S	0.646953	-1.363357	-1.299408
C	2.411780	0.608225	-0.419025
H	2.643491	1.392332	0.308708
H	2.272141	1.072717	-1.400357
H	3.266299	-0.074092	-0.476045
C	1.402549	-0.880695	1.353328
H	1.718530	-0.175775	2.129654
H	2.193588	-1.623051	1.218251
H	0.507795	-1.402157	1.711124
C	-0.170108	1.543081	1.477803
O	0.695016	2.289070	1.870369
O	-1.265698	1.260278	2.202084
H	-1.825281	0.670472	1.654825
H	-1.919598	-1.273385	-2.781877

Penone

C	-0.759279	2.639190	-1.427747
H	-1.257265	3.565240	-1.114280
C	-1.273136	1.391176	-0.649993
H	-2.232647	1.509759	-0.144165
C	0.587126	2.447211	-0.714040
O	1.704307	2.850332	-0.902803
C	0.717166	0.039852	0.307691
H	1.561751	0.062660	-0.393777
C	-0.285895	-1.061570	-0.201354
S	-1.194981	-0.185923	-1.579405
C	0.436044	-2.278349	-0.792562
H	0.976745	-2.819982	-0.006684
H	1.143598	-1.984562	-1.575588
H	-0.279109	-2.981113	-1.233056
C	-1.276198	-1.501297	0.889233
H	-0.760945	-2.045663	1.689833
H	-2.034364	-2.161319	0.458256
H	-1.787170	-0.649351	1.348040
C	0.002541	1.398071	0.254381
H	-0.170692	1.798904	1.258550

C	1.253588	-0.274366	1.707659
O	0.792137	0.168843	2.729749
O	2.289112	-1.154526	1.755148
H	2.588458	-1.370357	0.856902
H	-0.740893	2.597140	-2.519985

Penane

C	-0.787900	2.421528	-1.234074
H	-1.187785	3.437732	-1.300970
C	-1.058519	1.666991	0.099834
H	-1.370908	2.330157	0.910121
C	0.536865	-0.221873	-0.238521
H	0.389760	-0.306343	-1.324822
C	-0.656351	-0.985357	0.430866
S	-2.103814	0.153327	0.084909
C	-0.935037	-2.342571	-0.228416
H	-0.117082	-3.044108	-0.022801
H	-1.062435	-2.244094	-1.312733
H	-1.851012	-2.789435	0.172385
C	-0.468191	-1.159095	1.947055
H	0.374411	-1.826586	2.166422
H	-1.371864	-1.591121	2.387362
H	-0.275978	-0.204475	2.443410
C	0.441686	1.255546	0.160979
C	0.738296	2.288815	-0.963920
H	1.179732	3.208495	-0.569825
H	0.957540	1.416303	1.110009
H	1.361232	1.940424	-1.795102
C	1.895458	-0.830521	0.118657
O	2.604294	-0.446422	1.015154
O	2.278630	-1.901146	-0.632538
H	1.613119	-2.081971	-1.316229
H	-1.124148	1.855799	-2.107214

2,2-Dimethylpenam-3-carboxylic acid 27_{ax} NHB

Penamine

C	0.933088	-2.374136	-1.464118
H	1.103784	-3.429021	-1.232009
C	1.262586	-1.450990	-0.268934
H	1.927388	-1.817500	0.515475
N	-0.156999	-1.402531	0.070083
C	-0.613107	-0.117195	0.555761
H	-1.675035	0.001324	0.320203
C	0.198824	1.079515	-0.110882
S	1.787667	0.294993	-0.704410
C	-0.592162	1.663039	-1.296788
H	-1.517367	2.133040	-0.937224
H	-0.858282	0.900889	-2.032791
H	-0.004459	2.430955	-1.810527
C	0.533045	2.219362	0.869002
H	-0.386846	2.675499	1.255754
H	1.102162	3.001421	0.355939
H	1.134747	1.864374	1.709273
C	-0.540873	-1.938163	-1.261515
H	-0.863361	-1.178598	-1.983232
H	-1.296748	-2.729216	-1.211061
C	-0.469113	-0.112332	2.076382
O	0.455414	-0.579834	2.699986
O	-1.520600	0.504878	2.672755
H	-1.338881	0.483207	3.632073
H	1.395129	-2.122979	-2.419193

Lactam

C	-2.394977	-0.977675	-1.505864
H	-3.425051	-1.324179	-1.381487
C	-1.418990	-1.364357	-0.359047
H	-1.775468	-2.071179	0.390403
C	-2.136589	0.475274	-1.052573
O	-2.369020	1.584680	-1.462111
N	-1.422286	0.035368	0.071998
C	-0.194380	0.574875	0.608473
H	-0.189567	1.657116	0.455027
C	0.999436	-0.075719	-0.205592
S	0.345199	-1.747746	-0.774493
C	1.322622	0.809780	-1.422411
H	1.774469	1.754009	-1.090497
H	0.430188	1.049727	-2.007439
H	2.035478	0.305823	-2.082323
C	2.268685	-0.301012	0.627897
H	2.649285	0.654685	1.006255
H	3.050604	-0.750788	0.007599
H	2.086268	-0.969513	1.473492
C	-0.121449	0.287477	2.104996
O	-0.567945	-0.693471	2.652298
O	0.532598	1.274215	2.761505
H	0.565333	1.007516	3.700334
H	-2.044442	-1.194905	-2.516440

Penone

C	0.746559	-2.184949	-1.749432
H	0.904017	-3.268468	-1.826747
C	1.184700	-1.583548	-0.377212
H	1.812591	-2.223950	0.242617
C	-0.702827	-1.835505	-1.377239
O	-1.747749	-1.821582	-1.974799
C	-0.662546	-0.056998	0.596596
H	-1.695590	0.198889	0.334233
C	0.283995	1.006108	-0.079611
S	1.898698	0.102268	-0.388970
C	-0.332590	1.491501	-1.404159
H	-1.247141	2.066375	-1.206138
H	-0.594236	0.667607	-2.071587
H	0.371581	2.141755	-1.932097
C	0.600765	2.225442	0.800236
H	-0.315653	2.777040	1.036445
H	1.274850	2.903876	0.266334
H	1.088128	1.938047	1.735680
C	-0.305534	-1.448880	0.064030
H	-0.610081	-2.232617	0.766787
C	-0.567038	-0.053374	2.115121
O	0.143799	-0.772212	2.781910
O	-1.401680	0.861717	2.667866
H	-1.263277	0.808681	3.632928
H	1.136259	-1.707223	-2.652792

Penane

C	-1.138872	2.205456	-1.145487
H	-1.273817	3.281096	-1.298462
C	-0.656983	1.830692	0.287648
H	-0.535708	2.676961	0.967349
C	0.845808	-0.239946	0.044709
H	1.241012	-0.792864	-0.815253
C	-0.543244	-0.883989	0.429093
S	-1.518929	0.507297	1.204673
C	-1.255243	-1.420431	-0.827109
H	-0.667767	-2.228215	-1.284811

H	-1.412246	-0.644771	-1.579717
H	-2.236883	-1.824399	-0.559793
C	-0.447208	-2.016271	1.464710
H	0.142521	-2.851263	1.070469
H	-1.448776	-2.391879	1.699822
H	0.008714	-1.674541	2.397987
C	0.667119	1.251325	-0.305469
C	0.181062	1.630882	-1.736121
H	0.816305	2.372981	-2.228867
H	1.551944	1.809947	0.007562
H	0.057793	0.788991	-2.424032
C	1.864170	-0.386201	1.164839
O	2.058711	0.402343	2.062865
O	2.574122	-1.539819	1.048994
H	3.179924	-1.559715	1.814417
H	-2.053529	1.696332	-1.460015

2,2-Dimethylpenam-3-carboxylic acid 27_{eq} NHB

Penamine

C	0.227647	-2.550468	-1.654678
H	0.841023	-3.445202	-1.521246
C	0.908852	-1.281033	-1.097880
H	1.984605	-1.328235	-0.903570
N	0.055792	-1.341719	0.095491
C	-0.498270	-0.065577	0.517049
H	-1.572710	-0.028200	0.289982
C	0.193590	1.104232	-0.288809
S	0.508206	0.316679	-1.953330
C	-0.746178	2.301995	-0.469711
H	-1.010172	2.725814	0.504855
H	-1.668348	2.008462	-0.980707
H	-0.261000	3.086604	-1.060006
C	1.522184	1.550424	0.344667
H	1.345703	2.048366	1.306572
H	2.028547	2.259546	-0.316591
H	2.195533	0.708021	0.528142
C	-0.829633	-2.349410	-0.540012
H	-1.774804	-1.926224	-0.910872
H	-1.049953	-3.211890	0.097821
C	-0.350895	0.139092	2.026269
O	0.472317	-0.366386	2.749534
O	-1.283555	1.021330	2.483307
H	-1.107257	1.125033	3.437681
H	-0.131226	-2.501254	-2.683960

Lactam

C	0.573246	-2.434891	-1.923236
H	0.776939	-3.497994	-1.769067
C	1.057649	-1.502466	-0.781289
H	1.704057	-1.942595	-0.019253
C	-0.839550	-1.974081	-1.508360
O	-1.954140	-2.032099	-1.959939
N	-0.342819	-1.321124	-0.371142
C	-0.766237	-0.009107	0.080668
H	-1.513221	0.376859	-0.622420
C	0.503088	0.938453	0.066934
S	1.616777	0.188869	-1.246622
C	0.126579	2.363873	-0.352748
H	-0.571505	2.793101	0.374039
H	-0.346647	2.376502	-1.339252
H	1.014980	3.003191	-0.385436
C	1.239233	0.949021	1.417685
H	0.621084	1.425587	2.188536
H	2.167166	1.520625	1.328873
H	1.486654	-0.059598	1.761305
C	-1.416383	-0.067719	1.462502
O	-1.285601	-0.947257	2.277374
O	-2.168356	1.042211	1.678983
H	-2.539024	0.950858	2.577453
H	0.856033	-2.140221	-2.935589

Penone

C	-0.759279	2.639190	-1.427747
H	-1.257265	3.565240	-1.114280
C	-1.273136	1.391176	-0.649993
H	-2.232647	1.509759	-0.144165
C	0.587126	2.447211	-0.714040
O	1.704307	2.850332	-0.902803
C	0.717166	0.039852	0.307691
H	1.561751	0.062660	-0.393777
C	-0.285895	-1.061570	-0.201354
S	-1.194981	-0.185923	-1.579405
C	0.436044	-2.278349	-0.792562
H	0.976745	-2.819982	-0.006684
H	1.143598	-1.984562	-1.575588
H	-0.279109	-2.981113	-1.233056
C	-1.276198	-1.501297	0.889233
H	-0.760945	-2.045663	1.689833
H	-2.034364	-2.161319	0.458256
H	-1.787170	-0.649351	1.348040
C	0.002541	1.398071	0.254381
H	-0.170692	1.798904	1.258550
C	1.253588	-0.274366	1.707659
O	0.792137	0.168843	2.729749
O	2.289112	-1.154526	1.755148
H	2.588458	-1.370357	0.856902
H	-0.740893	2.597140	-2.519985

Penane

C	-0.787900	2.421528	-1.234074
H	-1.187785	3.437732	-1.300970
C	-1.058519	1.666991	0.099834
H	-1.370908	2.330157	0.910121
C	0.536865	-0.221873	-0.238521
H	0.389760	-0.306343	-1.324822
C	-0.656351	-0.985357	0.430866
S	-2.103814	0.153327	0.084909
C	-0.935037	-2.342571	-0.228416
H	-0.117082	-3.044108	-0.022801
H	-1.062435	-2.244094	-1.312733
H	-1.851012	-2.789435	0.172385
C	-0.468191	-1.159095	1.947055
H	0.374411	-1.826586	2.166422
H	-1.371864	-1.591121	2.387362
H	-0.275978	-0.204475	2.443410
C	0.441686	1.255546	0.160979
C	0.738296	2.288815	-0.963920
H	1.179732	3.208495	-0.569825
H	0.957540	1.416303	1.110009
H	1.361232	1.940424	-1.795102
C	1.895458	-0.830521	0.118657
O	2.604294	-0.446422	1.015154
O	2.278630	-1.901146	-0.632538
H	1.613119	-2.081971	-1.316229
H	-1.124148	1.855799	-2.107214

6-Acetamido-2,2-dimethyl-penam 28_{ax}

Penamine

C	-0.245784	1.706516	-0.160140
H	-0.417784	2.767480	0.025943
C	-0.639063	0.826239	1.061535
H	-1.351306	1.239240	1.781465
N	0.761136	0.791480	1.470979
C	1.172336	-0.495222	1.997410
H	0.947561	-0.515847	3.071384
H	2.257474	-0.605924	1.887941
C	0.423128	-1.691932	1.311921
S	-1.172082	-0.936472	0.684304
C	1.223810	-2.312309	0.153524
H	2.156832	-2.748571	0.534839
H	1.482615	-1.578773	-0.613966
H	0.655611	-3.114317	-0.330073
C	0.097256	-2.781310	2.346287
H	1.027045	-3.197735	2.756502
H	-0.463503	-3.606787	1.895251
H	-0.496098	-2.380076	3.173266
N	-0.813593	1.398511	-1.439805
H	-0.954742	0.419570	-1.654150
C	-1.269924	2.363221	-2.302677
O	-1.185280	3.561270	-2.065495
C	-1.874165	1.837841	-3.596611
H	-2.862120	2.287640	-3.730702
H	-1.968168	0.747873	-3.630083
H	-1.250823	2.164921	-4.435389
C	1.218116	1.279031	0.144081
H	1.575198	0.497688	-0.538161
H	1.966317	2.076755	0.200618

Lactam

C	-0.209052	1.739802	-0.185856
H	-0.370209	2.808590	-0.019931
C	-0.607979	0.870034	1.056494
H	-1.249657	1.338136	1.805775
C	1.237157	1.278450	0.164051
O	2.311025	1.256664	-0.381767
N	0.810555	0.777288	1.403640
C	1.235433	-0.464252	2.021652
H	1.027427	-0.424039	3.096546
H	2.314374	-0.577803	1.879049
C	0.453874	-1.644231	1.359508
S	-1.164770	-0.875365	0.760903
C	1.230068	-2.221850	0.164771
H	2.138388	-2.725238	0.521442
H	1.533875	-1.442151	-0.539365
H	0.627684	-2.958790	-0.376573
C	0.142165	-2.743762	2.382485
H	1.077741	-3.175832	2.760940
H	-0.436616	-3.556161	1.930550
H	-0.427777	-2.351855	3.230126
N	-0.731257	1.429681	-1.475027
H	-0.697129	0.468069	-1.784102
C	-1.318653	2.385569	-2.274229
O	-1.431037	3.552265	-1.927795
C	-1.787643	1.888614	-3.631168
H	-2.754948	2.344388	-3.854430
H	-1.874991	0.799198	-3.692057
H	-1.078050	2.224579	-4.395631

Penone

C	-0.215220	1.658942	-0.280708
H	-0.356525	2.735064	-0.118224
C	-0.675747	0.854661	0.987920
H	-1.433225	1.342606	1.602617
C	1.228511	1.255735	0.092788
O	2.261793	1.167864	-0.517576
C	1.203743	-0.544801	2.041759
H	0.950807	-0.603013	3.106665
H	2.288985	-0.680735	1.955473
C	0.463807	-1.670352	1.273369
S	-1.153685	-0.893307	0.690289
C	1.270858	-2.183334	0.067831
H	2.179389	-2.689151	0.420734
H	1.577304	-1.376786	-0.602006
H	0.687287	-2.907709	-0.510400
C	0.123067	-2.846688	2.200958
H	1.047891	-3.306388	2.573154
H	-0.440573	-3.621743	1.670127
H	-0.472265	-2.519025	3.058386
N	-0.736372	1.366911	-1.576142
H	-0.735633	0.399702	-1.872654
C	-1.360248	2.318996	-2.350775
O	-1.460377	3.485849	-1.998986
C	-1.905773	1.797170	-3.670618
H	-2.329794	2.632124	-4.229033
H	-2.686435	1.046541	-3.497923
H	-1.114246	1.327289	-4.265467
C	0.790254	0.827405	1.513557
H	1.002421	1.626175	2.234884

Penane

C	0.055159	1.674840	-0.312696
H	0.253855	2.749047	-0.320751
C	0.423282	1.050024	1.070285
H	0.478996	1.753951	1.904253
C	2.023620	-0.928425	0.840115
H	2.597955	-0.941015	1.774411
H	2.634494	-1.436958	0.082355
C	0.703304	-1.714301	1.070222
S	-0.538725	-0.413319	1.628390
C	0.192334	-2.437800	-0.187701
H	0.921136	-3.194428	-0.508155
H	0.021377	-1.758560	-1.026330
H	-0.751802	-2.951816	0.022249
C	0.864804	-2.740668	2.203154
H	1.606582	-3.497464	1.916513
H	-0.077027	-3.262003	2.407823
H	1.197943	-2.262488	3.129151
N	-1.285795	1.493989	-0.799419
H	-1.758693	0.640138	-0.530520
C	-1.945697	2.447698	-1.526976
O	-1.434248	3.515487	-1.843261
C	-3.368981	2.089015	-1.930551
H	-3.707412	1.120090	-1.549727
H	-3.434184	2.083116	-3.023374
H	-4.044512	2.870352	-1.569344
C	1.758121	0.528009	0.453684
C	1.226320	0.883023	-0.965587
H	1.896211	1.466571	-1.604142
H	2.610100	1.158419	0.729306
H	0.881483	0.015476	-1.533377

6-Acetamido-2,2-dimethyl-penam 28_{eq}

Penamine

C	0.261777	1.553055	-0.628452
H	0.224400	2.636427	-0.510407
C	-0.314722	0.816951	0.613594
H	-0.965504	1.392206	1.279288
N	1.052257	0.585125	1.101998
C	1.279723	-0.765476	1.622747
H	1.738871	-0.730198	2.620132
H	1.976179	-1.300441	0.962428
C	-0.063143	-1.544120	1.713106
S	-1.077869	-0.850990	0.302412
C	0.142202	-3.049038	1.510281
H	0.804935	-3.444473	2.290506
H	0.591994	-3.262006	0.535412
H	-0.806042	-3.593132	1.577474
C	-0.771003	-1.270800	3.050931
H	-0.173584	-1.670728	3.880853
H	-1.756042	-1.746916	3.077264
H	-0.907687	-0.198626	3.225443
N	-0.265569	1.256584	-1.929463
H	-0.386785	0.283002	-2.174087
C	-0.676875	2.232947	-2.803974
O	-0.598146	3.427553	-2.550494
C	-1.224702	1.725762	-4.129362
H	-1.293504	0.635433	-4.193672
H	-0.581022	2.089164	-4.937057
H	-2.217710	2.157036	-4.286165
C	1.627501	0.942961	-0.218481
H	1.896335	0.068019	-0.830437
H	2.483734	1.624721	-0.171820

Lactam

C	0.202650	1.611468	-0.649569
H	0.185827	2.698284	-0.534305
C	-0.270057	0.871887	0.646590
H	-0.818906	1.457553	1.387401
C	1.577402	0.969483	-0.312530
O	2.605236	0.741654	-0.897915
N	1.140329	0.606222	0.967591
C	1.458884	-0.670574	1.599062
H	1.873879	-0.525093	2.602876
C	0.150157	-1.523777	1.694917
S	-1.017169	-0.797149	0.412816
C	0.415028	-2.994910	1.354055
H	1.127891	-3.420302	2.071666
H	0.831572	-3.103564	0.347907
H	-0.504597	-3.586899	1.413205
C	-0.478830	-1.396507	3.091932
H	0.195077	-1.820023	3.848550
H	-1.430779	-1.933114	3.142541
H	-0.666030	-0.350164	3.355888
N	-0.386425	1.307420	-1.912592
H	-0.334147	0.355086	-2.246576
C	-0.942049	2.284125	-2.710232
O	-1.012761	3.453053	-2.360278
C	-1.438861	1.804327	-4.063088
H	-1.561232	0.718366	-4.123152
H	-0.726606	2.118802	-4.834096
H	-2.393982	2.289868	-4.276911
H	2.218500	-1.165523	0.984246

Penone

C	0.221713	1.491083	-0.784298
H	0.229041	2.584261	-0.695512
C	-0.340334	0.853636	0.534134
H	-1.014805	1.486247	1.113719
C	1.586267	0.899663	-0.380323
O	2.561919	0.559591	-0.995400
C	1.367917	-0.762811	1.625557
H	1.848575	-0.729915	2.610557
H	2.053010	-1.293095	0.953995
C	0.023140	-1.528678	1.723346
S	-1.009669	-0.839475	0.316952
C	0.199422	-3.036200	1.512673
H	0.833329	-3.452131	2.305888
H	0.672172	-3.248971	0.548738
H	-0.761546	-3.561472	1.548430
C	-0.676935	-1.248058	3.062685
H	-0.076284	-1.645568	3.891526
H	-1.663299	-1.720570	3.098007
H	-0.812686	-0.174629	3.232533
N	-0.328126	1.181948	-2.065452
H	-0.278982	0.222720	-2.380114
C	-0.822305	2.155145	-2.902824
O	-0.870156	3.333865	-2.578890
C	-1.286695	1.665307	-4.263883
H	-2.254445	2.120979	-4.488683
H	-1.374505	0.576709	-4.331152
H	-0.575969	2.007950	-5.024026
C	1.114240	0.649538	1.069649
H	1.435993	1.452931	1.742169

Penane

C	-1.849510	-0.025476	-0.477278
H	-2.936862	-0.146783	-0.495140
C	-1.274125	0.472361	0.895030
H	-2.075284	0.810257	1.555473
C	0.969014	1.241009	0.109573
H	1.601236	2.114725	-0.097748
C	1.375331	0.589456	1.447520
S	-0.075058	-0.546780	1.842323
C	2.650706	-0.251715	1.326611
H	3.502882	0.392532	1.075209
H	2.554370	-1.013677	0.546541
H	2.886025	-0.755990	2.270536
C	1.526365	1.632090	2.566339
H	2.365126	2.305153	2.342239
H	1.725464	1.150605	3.529098
H	0.623554	2.240597	2.678339
N	-1.228176	-1.232230	-0.972437
H	-0.564118	-1.694865	-0.361570
C	-1.623276	-1.799018	-2.149425
O	-2.472558	-1.283818	-2.869015
C	-0.946642	-3.115261	-2.507080
H	-0.124472	-3.384794	-1.835892
H	-0.566477	-3.049927	-3.530674
H	-1.693929	-3.915667	-2.487459
C	-0.520053	1.618611	0.159074
C	-1.350208	1.305951	-1.117953
H	-2.168434	2.012891	-1.282360
H	-0.663662	2.614860	0.588972
H	-0.790640	1.194113	-2.050389
H	1.143414	0.520790	-0.698458

6-Acetamido-2,2-dimethylpenam-3-carboxylic acid 15_{ax} HB

Penamine

C	-0.398572	1.709427	-0.495169
H	-0.670800	2.753297	-0.331483
C	-0.808607	0.794497	0.700674
H	-1.534537	1.215128	1.401977
N	0.593545	0.796311	1.171514
C	1.099246	-0.502248	1.622907
H	2.147501	-0.577387	1.309591
C	0.313506	-1.699493	0.948891
S	-1.296360	-0.945971	0.337691
C	1.115156	-2.249312	-0.246324
H	2.045987	-2.708460	0.110476
H	1.371368	-1.469068	-0.968959
H	0.542708	-3.019125	-0.773781
C	-0.050285	-2.866327	1.882255
H	0.854385	-3.346977	2.263116
H	-0.631615	-3.608313	1.323777
H	-0.643445	-2.539190	2.737928
N	-0.853129	1.355201	-1.806219
H	-0.934232	0.367851	-2.014942
C	-1.369002	2.283342	-2.681323
O	-1.390711	3.481078	-2.434296
C	-1.905206	1.713627	-3.984737
H	-1.404047	2.212134	-4.819837
H	-2.971758	1.948432	-4.058416
H	-1.772402	0.631595	-4.081752
C	1.074108	1.407488	-0.101955
H	1.565037	0.698373	-0.778529
H	1.729703	2.270551	0.048996
C	1.167075	-0.522250	3.173954
O	1.561906	-1.473609	3.805036
O	0.816443	0.637723	3.746955
H	0.637034	1.251672	2.991988

Lactam

C	-0.550337	1.685892	-0.438747
H	-0.901437	2.696090	-0.205366
C	-0.908917	0.650852	0.684751
H	-1.678349	0.953806	1.397975
C	0.914803	1.444806	0.015523
O	2.020054	1.640515	-0.410859
N	0.479117	0.756301	1.179889
C	1.094075	-0.464944	1.697100
H	2.169611	-0.388011	1.498907
C	0.527801	-1.688833	0.873384
S	-1.149158	-1.108859	0.213426
C	1.469865	-1.983089	-0.309247
H	2.418664	-2.388276	0.065596
H	1.694752	-1.088659	-0.897145
H	1.025670	-2.728535	-0.976020
C	0.291457	-2.980212	1.668215
H	1.234137	-3.347963	2.081706
H	-0.115206	-3.746438	0.998963
H	-0.406575	-2.838613	2.494329
N	-0.901574	1.423484	-1.792167
H	-0.713614	0.502573	-2.164665
C	-1.576346	2.352389	-2.559204
O	-1.890719	3.449737	-2.125121
C	-1.859491	1.917537	-3.985740
H	-1.118105	2.374929	-4.650695
H	-2.843715	2.290319	-4.277995
H	-1.824609	0.832166	-4.122184
C	0.967694	-0.536710	3.236618
O	1.338247	-1.485542	3.881519
O	0.467945	0.570294	3.816894
H	0.324261	1.232994	3.110359

Penone

C	-0.110798	1.687330	-0.668187
H	-0.169899	2.783728	-0.644739
C	-0.562409	1.092955	0.714825
H	-1.183199	1.761532	1.312773
C	1.327426	1.235503	-0.318162
O	2.342751	1.098263	-0.945082
C	1.219659	-0.503731	1.682127
H	2.261952	-0.768430	1.479399
C	0.279332	-1.524782	0.962136
S	-1.335518	-0.575495	0.725599
C	0.847804	-1.966972	-0.397683
H	1.791931	-2.506140	-0.249585
H	1.052459	-1.135650	-1.074427
H	0.145511	-2.645101	-0.893210
C	-0.013609	-2.783818	1.795495
H	0.920566	-3.327478	1.979472
H	-0.686906	-3.454730	1.252043
H	-0.468224	-2.553664	2.761207
N	-0.723861	1.278280	-1.889418
H	-0.830334	0.288494	-2.063237
C	-1.277135	2.188381	-2.765738
O	-1.246909	3.392012	-2.557381
C	-1.887119	1.586895	-4.019386
H	-2.796615	2.139294	-4.265801
H	-2.122127	0.522386	-3.921027
H	-1.185387	1.712035	-4.851771
C	0.927519	0.913043	1.143671
H	1.293430	1.687156	1.828072
C	1.095098	-0.490096	3.214906
O	2.043640	-0.630062	3.945781
O	-0.138929	-0.248091	3.721710
H	-0.810102	-0.253046	3.005619

Penane

C	-0.126888	1.726631	-0.619004
H	-0.004215	2.806679	-0.729533
C	0.347701	1.245371	0.789400
H	0.504402	2.052944	1.508613
C	1.790916	-0.869196	0.555210
H	2.255657	-1.440980	-0.254215
C	0.398940	-1.502922	0.893276
S	-0.568656	-0.083525	1.669142
C	-0.328880	-2.028596	-0.357711
H	0.282759	-2.791576	-0.855970
H	-0.552260	-1.246526	-1.084549
H	-1.276345	-2.495670	-0.068721
C	0.480252	-2.651105	1.915310
H	1.067667	-3.475947	1.494766
H	-0.520394	-3.035836	2.137595
H	0.945448	-2.348724	2.855854
N	-1.478515	1.414794	-1.004930
H	-1.941576	0.656971	-0.519536
C	-2.197249	2.227372	-1.846365
O	-1.710732	3.219491	-2.372620
C	-3.638617	1.805696	-2.087650
H	-3.921441	0.882429	-1.572579
H	-3.790084	1.673218	-3.163169
H	-4.302175	2.613014	-1.762351

C	1.619671	0.611681	0.137773
C	1.061070	0.954626	-1.274249
H	1.719023	1.572870	-1.890863
H	2.531794	1.172607	0.362006
H	0.753941	0.090449	-1.866372
C	2.797493	-0.935194	1.713840
O	3.886056	-1.444131	1.610138
O	2.428629	-0.324131	2.867949
H	1.486607	-0.052785	2.819514

6-Acetamido-2,2-dimethylpenam-3-carboxylic acid 15_{eq} HB

Penamine

N	-0.376450	-0.133538	-1.248727
C	0.724084	-0.616700	-0.371507
H	1.150056	-1.580600	-0.662544
C	1.558438	0.647897	-0.730433
H	2.322130	0.423680	-1.475990
C	3.560734	1.639825	0.310372
O	4.291153	1.291010	-0.604988
N	2.204847	1.386346	0.312827
H	1.649578	1.654767	1.114778
S	0.047052	-0.707604	1.339968
C	-1.633529	-1.143061	0.637980
C	-1.712061	-0.234393	-0.634157
H	-2.057731	0.757801	-0.319480
C	-2.726357	-0.782084	1.649363
H	-2.653054	0.265196	1.960618
H	-2.655782	-1.413958	2.540700
H	-3.706540	-0.938427	1.188543
C	-1.687374	-2.642944	0.299021
H	-1.511417	-3.237173	1.199947
H	-0.937386	-2.927499	-0.446054
H	-2.675707	-2.902814	-0.096242
C	-2.746238	-0.763640	-1.648809
O	-3.931863	-0.805489	-1.412257
O	-2.209267	-1.188405	-2.800974
H	-1.241395	-0.999154	-2.713241
C	4.059296	2.398470	1.529923
H	3.826903	1.856469	2.454116
H	3.589251	3.386770	1.594487
H	5.139690	2.521309	1.446382
C	0.255208	1.217741	-1.346933
H	-0.232612	1.959000	-0.700483
H	0.316343	1.611203	-2.366204

Lactam

C	0.276499	1.258840	-1.196754
O	-0.165118	2.353301	-1.414007
N	-0.360435	-0.013731	-1.207730
C	0.726323	-0.615026	-0.387980
H	1.108340	-1.566527	-0.762159
C	1.598739	0.653593	-0.667056
H	2.335117	0.476206	-1.456600
C	3.624272	1.598121	0.330010
O	4.320284	1.211231	-0.595687
N	2.270775	1.327494	0.392338
H	1.719172	1.689554	1.158151
S	0.015704	-0.772208	1.295312
C	-1.679000	-1.115743	0.557251
C	-1.731728	-0.170463	-0.696019
H	-2.096254	0.816644	-0.390364
C	-2.764359	-0.747527	1.573174
H	-2.665350	0.290637	1.906052
H	-2.713476	-1.400693	2.450459
H	-3.746284	-0.870869	1.105645
C	-1.774382	-2.603395	0.176367
H	-1.624371	-3.225899	1.062574
H	-1.023474	-2.888775	-0.568540
H	-2.764683	-2.824005	-0.235755
C	-2.713299	-0.681831	-1.765034
O	-3.894551	-0.801687	-1.542997
O	-2.163700	-0.995585	-2.949433
H	-1.209996	-0.776143	-2.893516
C	4.162412	2.433594	1.476821
H	5.190614	2.128592	1.680892
H	3.565254	2.344883	2.389788
H	4.176952	3.487419	1.174801

Penone

C	0.075185	1.630274	-0.846674
O	-0.760102	2.491258	-0.932839
C	1.129144	-0.097731	-0.169567
H	2.030940	-0.671259	-0.388611
C	1.338390	1.446880	0.016932
H	2.232929	1.765827	-0.531742
C	2.503649	2.763346	1.731402
O	3.501412	2.892741	1.037338
N	1.404738	2.046362	1.310277
H	0.590287	1.977242	1.905581
S	0.119160	-0.880918	1.142200
C	-1.032540	-1.696692	-0.087786
C	-1.182676	-0.617354	-1.221989
H	-1.984447	0.069068	-0.925039
C	-2.357918	-1.992643	0.623518
H	-2.809425	-1.077098	1.018117
H	-2.202840	-2.686646	1.456890
H	-3.065005	-2.454089	-0.073165
C	-0.394982	-2.996619	-0.605543
H	-0.197733	-3.676785	0.227895
H	0.549781	-2.813612	-1.126924
H	-1.073028	-3.503828	-1.303270
C	2.360897	3.389760	3.108476
H	1.947008	2.683183	3.836623
H	1.690056	4.256021	3.059878
H	3.342879	3.726014	3.443571
C	-1.599805	-1.227210	-2.553039
O	-0.890990	-1.379909	-3.522857
O	-2.900721	-1.610060	-2.539313
H	-3.081002	-1.995922	-3.417902
C	0.132260	0.168526	-1.340254
H	0.584496	0.071873	-2.332186

Penane

C	1.621012	-0.575552	-0.260405
H	2.513921	-1.104704	-0.599291
C	1.907270	0.952633	-0.057530
H	2.965202	1.221699	-0.124799
C	1.611043	2.801744	1.519461
O	2.249752	3.566189	0.804827
N	1.358443	1.508544	1.157320
H	0.877406	0.875213	1.785492
S	0.778314	-1.552161	1.046181
C	-0.786484	-1.782378	0.029398
C	-0.807805	-0.489147	-0.855754
H	-1.107752	0.335043	-0.199819

C	-1.984139	-1.865754	0.983152
H	-2.082934	-0.956566	1.584472
H	-1.876527	-2.717828	1.662846
H	-2.912631	-2.003661	0.417990
C	-0.666076	-3.071088	-0.798793
H	-0.556140	-3.933685	-0.134500
H	0.198990	-3.048158	-1.467463
H	-1.561636	-3.223969	-1.412957
C	1.055059	3.227104	2.871052
H	1.890105	3.437206	3.547868
H	0.404995	2.478857	3.335711
H	0.496614	4.159063	2.745181
C	-1.829243	-0.572758	-1.978065
O	-1.624988	-0.988014	-3.097738
O	-3.051246	-0.137932	-1.578690
H	-3.641877	-0.244555	-2.349076
C	0.610343	-0.240688	-1.393000
H	0.755101	-0.777448	-2.333158
C	1.105265	1.234003	-1.365907
H	1.755410	1.483721	-2.208448
H	0.335232	2.005027	-1.275558

6-Acetamido-2,2-dimethylpenam-3-carboxylic acid 14_{ax} NHB

Penamine

C	-0.207130	1.756178	-0.663294
H	-0.254498	2.830903	-0.483347
C	-0.627853	0.941858	0.593419
H	-1.267145	1.415614	1.339991
N	0.780300	0.797902	0.942179
C	1.117422	-0.481387	1.532034
H	2.167140	-0.708934	1.325033
C	0.211534	-1.651091	0.944296
S	-1.296921	-0.779514	0.258033
C	0.957625	-2.403272	-0.172942
H	1.832040	-2.922342	0.241322
H	1.303615	-1.735772	-0.965735
H	0.306977	-3.156720	-0.628816
C	-0.244685	-2.667987	2.006140
H	0.623192	-3.153816	2.468057
H	-0.856781	-3.448186	1.542695
H	-0.842904	-2.193373	2.787185
N	-0.867894	1.502919	-1.909161
H	-1.095697	0.540130	-2.122469
C	-1.311713	2.509774	-2.731433
O	-1.122383	3.694789	-2.491839
C	-2.046741	2.045790	-3.979922
H	-3.020699	2.542601	-4.018514
H	-2.196511	0.962714	-4.028469
H	-1.482077	2.365281	-4.861719
C	1.218567	1.182364	-0.422387
H	1.446256	0.340354	-1.087556
H	2.052429	1.891731	-0.437359
C	0.955194	-0.355246	3.046682
O	0.062261	0.231243	3.612564
O	1.946617	-1.004004	3.706646
H	1.760462	-0.890503	4.658687

Lactam

C	-0.462772	1.807604	-0.498094
H	-0.729337	2.839810	-0.253884
C	-0.848110	0.801535	0.641427
H	-1.563403	1.131527	1.394132
C	1.000547	1.450005	-0.099813
O	2.101294	1.570225	-0.573299
N	0.552174	0.805564	1.065269
C	1.071125	-0.424895	1.620727
H	2.156150	-0.438484	1.489677
C	0.430371	-1.624840	0.807350
S	-1.209316	-0.951207	0.160304
C	1.350964	-1.992678	-0.370107
H	2.274145	-2.452224	0.007079
H	1.629048	-1.118951	-0.965966
H	0.858988	-2.716130	-1.027998
C	0.148705	-2.872019	1.657416
H	1.082415	-3.260561	2.080044
H	-0.290182	-3.658992	1.035855
H	-0.548696	-2.660168	2.472034
N	-0.884074	1.565440	-1.837582
H	-0.762318	0.634655	-2.212457
C	-1.513453	2.531698	-2.592409
O	-1.737869	3.654478	-2.165993
C	-1.876113	2.104390	-4.004607
H	-1.138537	2.517038	-4.702144
H	-2.849112	2.530430	-4.259378
H	-1.907690	1.018075	-4.135622
C	0.751084	-0.480965	3.111790
O	-0.241465	-0.026821	3.631035
O	1.720593	-1.130807	3.795746
H	1.434846	-1.152732	4.729468

Penone

C	-0.320238	1.710434	-0.772837
H	-0.395297	2.796752	-0.636379
C	-0.728625	0.970978	0.551835
H	-1.423548	1.498781	1.204582
C	1.123149	1.242097	-0.484390
O	2.101912	1.058087	-1.159276
C	1.182891	-0.433254	1.575781
H	2.237366	-0.630561	1.353452
C	0.326463	-1.583752	0.921409
S	-1.269150	-0.768282	0.340128
C	1.079368	-2.189787	-0.276916
H	1.970694	-2.723552	0.077200
H	1.402865	-1.429707	-0.991136
H	0.443431	-2.908545	-0.803558
C	-0.057484	-2.711191	1.894724
H	0.840482	-3.218453	2.265365
H	-0.675574	-3.454747	1.380460
H	-0.629708	-2.334429	2.747240
N	-0.940956	1.408078	-2.020374
H	-0.989390	0.436480	-2.297341
C	-1.518621	2.378447	-2.808899
O	-1.520314	3.559952	-2.494365
C	-2.136702	1.858100	-4.096509
H	-2.618648	2.688098	-4.613821
H	-2.878667	1.077530	-3.892065
H	-1.367095	1.427247	-4.747740
C	0.761767	0.912521	0.983066
H	1.034199	1.747139	1.638897
C	1.032914	-0.385918	3.089254
O	0.209357	0.261631	3.697147
O	1.951226	-1.166651	3.708944
H	1.771936	-1.093522	4.666120

Penane

C	-0.359196	1.737043	-0.649108
H	-0.111348	2.800641	-0.628381
C	-0.000780	1.071904	0.715755
H	0.022751	1.717939	1.595335
C	1.747141	-0.806448	0.504671
H	2.308434	-1.295475	-0.299311
C	0.461919	-1.679573	0.793055
S	-0.931716	-0.459559	1.115476
C	0.124864	-2.564588	-0.420876
H	0.909802	-3.318895	-0.561471
H	0.037824	-1.988379	-1.344918
H	-0.822531	-3.089907	-0.261557
C	0.584533	-2.585243	2.033414
H	1.388732	-3.316992	1.895722
H	-0.348912	-3.136627	2.187471
H	0.783119	-2.004433	2.937648
N	-1.702806	1.642409	-1.148731
H	-2.152777	0.738700	-1.083610
C	-2.430593	2.736855	-1.542280
O	-1.966986	3.870035	-1.568500
C	-3.869490	2.446934	-1.944175
H	-4.541283	2.896205	-1.204884
H	-4.098993	1.379637	-2.024543
H	-4.069192	2.931397	-2.903803
C	1.347650	0.618452	0.094830
C	0.767656	0.903355	-1.320905
H	1.416604	1.429923	-2.027030
H	2.146460	1.324621	0.337841
H	0.372120	0.010396	-1.811399
C	2.664689	-0.740687	1.715564
O	2.605125	0.077000	2.607530
O	3.596639	-1.727512	1.697123
H	4.120545	-1.619128	2.514049

6-Acetamido-2,2-dimethylpenam-3-carboxylic acid 14_{eq} NHB

Penamine

N	0.117113	0.096437	-1.292502
C	1.070939	-0.144542	-0.201608
H	1.915168	-0.794888	-0.447378
C	1.350150	1.383834	-0.122311
H	2.275357	1.650048	-0.634457
C	2.445827	2.786146	1.584911
O	3.422792	3.010165	0.884060
N	1.380589	2.027540	1.159494
H	0.616340	1.844975	1.795823
S	0.105364	-0.880337	1.200651
C	-1.007300	-1.727898	-0.039058
C	-1.120728	-0.663196	-1.198392
H	-1.954635	0.008606	-0.953359
C	-2.365867	-2.005403	0.614742
H	-2.813350	-1.086401	1.005969
H	-2.259243	-2.714972	1.442058
H	-3.053041	-2.440605	-0.118498
C	-0.355094	-3.040272	-0.508926
H	-0.164114	-3.691010	0.349121
H	0.591931	-2.867947	-1.028475
H	-1.020834	-3.574789	-1.198007
C	2.319655	3.338124	2.996792
H	1.388396	3.059154	3.499113
H	2.391556	4.429307	2.956945
H	3.165056	2.977388	3.590748
C	-1.469502	-1.333254	-2.530453
O	-0.704749	-1.631414	-3.414032
O	-2.805918	-1.589901	-2.597577
H	-2.950404	-2.040147	-3.451493
C	0.090196	1.553264	-1.011153
H	0.188219	2.187029	-1.898854
H	-0.789869	1.874959	-0.433894

Lactam

C	0.019388	1.606462	-0.848337
O	-0.807569	2.467934	-0.999753
N	0.033741	0.259327	-1.239829
C	1.093872	-0.091362	-0.285226
H	1.911043	-0.691144	-0.690076
C	1.354714	1.438763	-0.072382
H	2.229582	1.788587	-0.626518
C	2.519480	2.721409	1.661914
O	3.496015	2.908000	0.951995
N	1.433767	1.981201	1.243729
H	0.637395	1.868196	1.855317
S	0.211104	-0.961236	1.077962
C	-1.038843	-1.667145	-0.135622
C	-1.156450	-0.569619	-1.275612
H	-2.019215	0.074736	-1.072966
C	-2.380535	-1.857227	0.582241
H	-2.745090	-0.915602	1.003628
H	-2.288091	-2.585782	1.394742
H	-3.128592	-2.233456	-0.124407
C	-0.514655	-3.013439	-0.664266
H	-0.352787	-3.702839	0.168913
H	0.430115	-2.903258	-1.204237
H	-1.245037	-3.469446	-1.343495
C	2.400851	3.301072	3.060719
H	3.341156	3.133130	3.592079
H	1.575941	2.877187	3.641480
H	2.254900	4.383950	2.982534
C	-1.364465	-1.201923	-2.650949
O	-0.518925	-1.374066	-3.493267
O	-2.659504	-1.580191	-2.803801
H	-2.723308	-1.992217	-3.686511

Penone

C	0.075185	1.630274	-0.846674
O	-0.760102	2.491258	-0.932839
C	1.129144	-0.097731	-0.169567
H	2.030940	-0.671259	-0.388611
C	1.338390	1.446880	0.016932
H	2.232929	1.765827	-0.531742
C	2.503649	2.763346	1.731402
O	3.501412	2.892741	1.037338
N	1.404738	2.046362	1.310277
H	0.590287	1.977242	1.905581
S	0.119160	-0.880918	1.142200
C	-1.032540	-1.696692	-0.087786
C	-1.182676	-0.617354	-1.221989
H	-1.984447	0.069068	-0.925039
C	-2.357918	-1.992643	0.623518
H	-2.809425	-1.077098	1.018117
H	-2.202840	-2.686646	1.456890
H	-3.065005	-2.454089	-0.073165
C	-0.394982	-2.996619	-0.605543
H	-0.197733	-3.676785	0.227895
H	0.549781	-2.813612	-1.126924

H	-1.073028	-3.503828	-1.303270
C	2.360897	3.389760	3.108476
H	1.947008	2.683183	3.836623
H	1.690056	4.256021	3.059878
H	3.342879	3.726014	3.443571
C	-1.599805	-1.227210	-2.553039
O	-0.890990	-1.379909	-3.522857
O	-2.900721	-1.610060	-2.539313
H	-3.081002	-1.995922	-3.417902
C	0.132260	0.168526	-1.340254
H	0.584496	0.071873	-2.332186

Penane

C	1.621012	-0.575552	-0.260405
H	2.513921	-1.104704	-0.599291
C	1.907270	0.952633	-0.057530
H	2.965202	1.221699	-0.124799
C	1.611043	2.801744	1.519461
O	2.249752	3.566189	0.804827
N	1.358443	1.508544	1.157320
H	0.877406	0.875213	1.785492
S	0.778314	-1.552161	1.046181
C	-0.786484	-1.782378	0.029398
C	-0.807805	-0.489147	-0.855754
H	-1.107752	0.335043	-0.199819
C	-1.984139	-1.865754	0.983152
H	-2.082934	-0.956566	1.584472
H	-1.876527	-2.717828	1.662846
H	-2.912631	-2.003661	0.417990
C	-0.666076	-3.071088	-0.798793
H	-0.556140	-3.933685	-0.134500
H	0.198990	-3.048158	-1.467463
H	-1.561636	-3.223969	-1.412957
C	1.055059	3.227104	2.871052
H	1.890105	3.437206	3.547868
H	0.404995	2.478857	3.335711
H	0.496614	4.159063	2.745181
C	-1.829243	-0.572758	-1.978065
O	-1.624988	-0.988014	-3.097738
O	-3.051246	-0.137932	-1.578690
H	-3.641877	-0.244555	-2.349076
C	0.610343	-0.240688	-1.393000
H	0.755101	-0.777448	-2.333158
C	1.105265	1.234003	-1.365907
H	1.755410	1.483721	-2.208448
H	0.335232	2.005027	-1.275558

6-Acetamido-2,2-dimethylpenam-3-carboxylate 16

Penamine

C	0.265198	0.440095	-1.767821
H	0.365061	0.235383	-2.834373
C	0.631905	-0.783663	-0.881805
H	1.302889	-1.562371	-1.241683
N	-0.767308	-1.124610	-0.802598
C	-1.161440	-1.733883	0.462240
H	-2.232770	-1.562759	0.614465
C	-0.364073	-1.052841	1.660757
S	1.179367	-0.321277	0.876358
C	-1.187474	0.058924	2.337592
H	-2.084701	-0.378387	2.796897
H	-1.512888	0.827510	1.630638
H	-0.614722	0.553944	3.132609
C	0.063806	-2.074949	2.727255
H	-0.821186	-2.602865	3.097402
H	0.568497	-1.579542	3.566902
H	0.732521	-2.816735	2.287694
N	0.918162	1.693919	-1.489369
H	1.120972	1.860760	-0.509687
C	1.277858	2.604005	-2.433282
O	1.071108	2.467786	-3.636845
C	1.969338	3.852471	-1.889725
H	2.937454	3.964128	-2.388446
H	2.126500	3.835686	-0.806313
H	1.366925	4.730027	-2.148028
C	-1.182366	0.223694	-1.240272
H	-1.425720	0.930349	-0.434446
H	-1.993484	0.230213	-1.979837
C	-0.912215	-3.295355	0.425052
O	-1.792939	-3.972321	1.003420
O	0.155725	-3.647335	-0.134753

Lactam

C	0.504613	0.296031	-1.802316
H	0.826294	0.042497	-2.814801
C	0.792659	-0.815995	-0.741660
H	1.467817	-1.633712	-0.984085
C	-0.993388	-0.049727	-1.501371
O	-2.066453	0.457780	-1.751832
N	-0.617830	-1.160632	-0.773055
C	-1.165347	-1.775790	0.428395
H	-2.251716	-1.657823	0.414777
C	-0.569494	-0.944615	1.634326
S	1.085191	-0.255034	1.009442
C	-1.497763	0.228228	1.995449
H	-2.425689	-0.164615	2.433617
H	-1.766901	0.822085	1.116034
H	-1.032208	0.893467	2.733264
C	-0.302153	-1.810133	2.871650
H	-1.226546	-2.317867	3.164442
H	0.055465	-1.194425	3.707053
H	0.441084	-2.577205	2.647114
N	0.943866	1.632007	-1.518952
H	0.860221	1.929393	-0.554409
C	1.521394	2.454254	-2.440662
O	1.714915	2.140593	-3.611034
C	1.900668	3.834842	-1.914611
H	1.211846	4.576153	-2.335556
H	2.906209	4.080824	-2.267697
H	1.871864	3.911889	-0.822640
C	-0.812037	-3.315064	0.521655
O	-1.667734	-3.987841	1.137143
O	0.291151	-3.639569	0.020319

Penone

C	-0.485156	1.746446	-0.529016
H	-0.874634	2.715407	-0.199021
C	-0.833406	0.614573	0.491496
H	-1.690363	0.815984	1.138226
C	0.992293	1.565337	-0.089230
O	2.035141	1.869430	-0.615651
C	1.310030	-0.626712	1.296571
H	2.110579	-0.712140	0.551725
C	0.290313	-1.773476	1.032961
S	-0.923580	-1.066479	-0.238360
C	0.973602	-3.012694	0.449647
H	1.759418	-3.298402	1.157155

H	1.437303	-2.791944	-0.518715
H	0.269848	-3.845169	0.319597
C	-0.499478	-2.151525	2.297226
H	0.191039	-2.603339	3.016445
H	-1.296571	-2.865313	2.060017
H	-0.946575	-1.271435	2.770372
N	-0.819393	1.603298	-1.918845
H	-0.517349	0.747307	-2.364742
C	-1.469769	2.553519	-2.648586
O	-1.868604	3.616702	-2.182233
C	-1.663118	2.210168	-4.121979
H	-2.711740	2.375423	-4.386770
H	-1.386591	1.181483	-4.374190
H	-1.059452	2.895152	-4.727810
C	0.596499	0.721111	1.118613
H	0.653441	1.254609	2.079334
C	1.994336	-0.778214	2.728365
O	2.637217	-1.847491	2.871729
O	1.794720	0.158385	3.535667

Penane

C	-0.279575	1.818710	-0.377320
H	-0.195673	2.860872	-0.063385
C	-0.147864	0.844069	0.833238
H	-0.275419	1.311369	1.814554
C	1.556988	-1.023916	0.287341
H	1.503934	-1.330680	-0.766525
C	0.414889	-1.782485	1.021077
S	-1.125503	-0.709664	0.745050
C	0.178412	-3.170041	0.420989
H	1.138210	-3.695406	0.471224
H	-0.126445	-3.098767	-0.629785
H	-0.590725	-3.730769	0.968804
C	0.663671	-1.894604	2.533625
H	1.545255	-2.523691	2.694539
H	-0.199084	-2.341718	3.041616
H	0.859050	-0.915507	2.983649
N	-1.474317	1.725089	-1.187746
H	-1.803593	0.784899	-1.370888
C	-2.186386	2.790958	-1.640024
O	-1.879200	3.963573	-1.434419
C	-3.426533	2.437507	-2.458440
H	-3.630080	1.363200	-2.515229
H	-3.303081	2.828759	-3.474073
H	-4.292507	2.941734	-2.018086
C	1.304423	0.487693	0.375778
C	1.050063	1.260731	-0.953348
H	1.791141	2.012511	-1.245760
H	2.087400	0.935505	0.992287
H	0.882728	0.587001	-1.801383
C	2.999741	-1.471218	0.804649
O	3.218151	-2.707365	0.716704
O	3.741926	-0.558350	1.231286

1-Azabicyclo[3.3.1]nonan-2-one 30 (Table 6)

1-Azabicyclo[3.3.1]nonane

H	0.535183	2.238590	-0.800243
C	0.252686	1.272583	-0.360616
C	-1.655571	0.076933	0.836573
N	-0.239789	-1.088479	-0.906182
C	-1.552432	-1.011034	-0.251831
C	0.100034	0.219781	-1.477363
C	-1.122892	1.428844	0.325727
H	-1.082213	-0.234368	1.719957
H	-2.294016	-0.809194	-1.037945
H	-0.700599	0.509839	-2.170584
H	-1.834714	1.849041	-0.400444
H	-2.697098	0.176358	1.169983
H	-1.796720	-1.996514	0.162643
H	1.012945	0.128725	-2.077124
H	-1.058678	2.148603	1.153159
C	1.940693	-0.569025	0.274390
H	2.594289	-0.464332	-0.600782
H	2.579829	-0.945309	1.083019
C	1.358731	0.808058	0.641220
H	0.946920	0.765239	1.657991
H	2.169947	1.544920	0.678932
C	0.841693	-1.606657	-0.032032
H	1.299652	-2.490130	-0.501479
H	0.402121	-1.952473	0.913033

1-Azabicyclo[3.3.1]nonan-2-one

H	0.512193	2.215694	-0.738314
C	0.293883	1.223095	-0.324442
C	-1.662086	-0.080945	0.794302
N	-0.149191	-1.100953	-0.842797
C	-1.529133	-1.135940	-0.324046
C	0.155933	0.197410	-1.458641
C	-1.082130	1.295095	0.389331
H	-1.132264	-0.464436	1.675202
H	-2.212812	-0.936071	-1.156985
H	-0.660043	0.452573	-2.143066
H	-1.785170	1.789538	-0.297121
H	-2.712907	0.032705	1.089178
H	-1.731562	-2.139010	0.053572
H	1.064316	0.119063	-2.063400
H	-1.012903	1.939737	1.275190
C	0.805636	-1.570492	0.064957
C	2.007709	-0.649544	0.219590
H	2.598159	-0.607104	-0.703531
H	2.648617	-1.055275	1.005118
C	1.481965	0.771552	0.582622
H	1.174605	0.772818	1.635261
H	2.308663	1.486095	0.504230
O	0.618522	-2.555605	0.763788

Bicyclo[3.3.1]nonan-2-one

C	0.002164	0.035074	-1.567528
C	0.299399	-1.171159	-0.662546
C	-0.928270	-1.475867	0.223489
C	-1.537064	1.014376	0.175334
C	-0.277088	1.271996	-0.692356
H	0.470349	-2.054541	-1.293004
H	-1.730474	-1.836800	-0.436673
H	-0.700860	-2.304783	0.907061
H	-1.734835	1.882895	0.815312
H	-2.387451	0.934948	-0.516536
H	-0.460482	2.157541	-1.310575
C	1.615723	-0.907967	0.101031
H	2.431703	-0.933230	-0.633646
H	1.814410	-1.724905	0.806443
C	1.674159	0.445669	0.846149
H	2.707245	0.763215	1.022058
H	1.218870	0.347354	1.840939
C	0.948363	1.604512	0.160616
C	-1.454756	-0.267766	1.023233

H	-0.823327	-0.093826	1.902997
H	-2.450052	-0.501256	1.422341
H	0.849897	0.224678	-2.239915
H	-0.868491	-0.163896	-2.207658
O	1.320868	2.753737	0.313432

Bicyclo[3.3.1]nonane

C	-0.000000	1.254189	0.670751
C	-0.000000	-1.254189	0.670751
C	1.307650	-1.284986	-0.153528
C	1.582697	-0.000000	-0.961505
C	1.307650	1.284986	-0.153528
H	2.135458	-1.435973	0.554881
H	1.316203	-2.155278	-0.823994
H	0.981764	-0.000000	-1.875590
H	2.628262	-0.000000	-1.297239
H	2.135458	1.435973	0.554881
C	-1.307650	-1.284986	-0.153528
H	-1.316203	-2.155278	-0.823994
H	-2.135458	-1.435973	0.554881
C	-1.307650	1.284986	-0.153528
H	-1.316203	2.155278	-0.823994
C	-1.582697	-0.000000	-0.961505
H	-0.981764	-0.000000	-1.875590
H	-2.628262	-0.000000	-1.297239
H	1.316203	2.155278	-0.823994
H	-2.135458	1.435973	0.554881
H	-0.000000	2.149115	1.309215
H	-0.000000	-2.149115	1.309215
C	-0.000000	0.000000	1.564421
H	-0.883718	0.000000	2.217441
H	0.883718	0.000000	2.217441

1-Aza-9,10-benzobicyclo[3.3.2]nonan-2-one 31 (Table 6)

1-Aza-9,10-benzobicyclo[3.3.2]decane

H	-0.072037	2.220349	1.183081
C	-0.145436	1.150654	0.950058
C	-1.949589	-0.729411	1.293594
N	-0.164268	-1.442442	-0.395409
C	-1.564709	-1.520180	0.030934
C	-1.622654	0.769766	1.249843
H	-1.459005	-1.184167	2.164681
H	-2.172693	-1.181817	-0.816741
H	-2.261552	1.265092	0.505831
H	-3.028036	-0.854315	1.466070
H	-1.812740	-2.579165	0.190582
H	-1.889859	1.204958	2.222909
C	1.667059	-0.740713	1.239531
H	2.336797	-0.318760	0.480504
H	2.319555	-1.192671	1.999223
C	0.873688	0.410430	1.881020
H	0.346778	0.051457	2.774988
H	1.605715	1.142864	2.244071
C	0.845886	-1.868615	0.587299
H	1.554991	-2.555322	0.100294
H	0.334036	-2.455557	1.359129
C	0.176018	-0.263438	-1.139628
C	0.841171	1.990173	-2.660309
C	0.194546	1.007687	-0.525251
C	0.498033	-0.390194	-2.492971
C	0.828457	0.730624	-3.257624
C	0.528737	2.120627	-1.304795
H	0.479468	-1.383855	-2.931732
H	1.071765	0.618703	-4.311040
H	0.545558	3.106129	-0.843461
H	1.094319	2.871110	-3.244680

1-Aza-9,10-benzobicyclo[3.3.2]decan-2-one

H	-0.191772	2.156384	1.197148
C	-0.162020	1.085445	0.959850
C	-1.940728	-0.922089	1.205599
N	-0.021632	-1.463079	-0.264795
C	-1.465354	-1.698425	-0.036461
C	-1.618347	0.589692	1.235532
H	-1.499474	-1.406492	2.083609
H	-1.993002	-1.385583	-0.941930
H	-2.266561	1.112623	0.518887
H	-3.027507	-1.043328	1.308326
H	-1.630108	-2.769068	0.105116
H	-1.906850	0.959632	2.228877
C	0.785867	-1.781735	0.830756
C	1.771186	-0.707814	1.251478
H	2.371964	-0.345822	0.411818
H	2.441678	-1.131729	2.002857
C	0.958919	0.468678	1.866791
H	0.513005	0.132918	2.811167
H	1.672391	1.260094	2.124500
O	0.573522	-2.776676	1.508216
C	0.285225	-0.312265	-1.072476
C	0.821560	1.912182	-2.659606
C	0.201054	0.969849	-0.507287
C	0.633392	-0.482674	-2.411918
C	0.901082	0.632730	-3.209555
C	0.477054	2.076041	-1.315010
H	0.693801	-1.489592	-2.814973
H	1.172164	0.500441	-4.253361
H	0.420645	3.075524	-0.888823
H	1.028844	2.784140	-3.274332

9,10-benzobicyclo[3.3.2]decan-2-one

C	0.552924	-1.207831	0.675843
C	-0.698399	-1.247623	1.590254
C	-1.664987	1.084115	0.886502
C	-0.553476	1.476562	-0.128808
H	0.925842	-2.240905	0.664538
H	-1.453349	-1.860833	1.079625
H	-0.432214	-1.792825	2.506505
H	-2.035922	2.007668	1.350333
H	-2.495210	0.686300	0.288362
H	-0.933217	2.343284	-0.678224
C	1.747865	-0.372449	1.202054
H	2.566872	-0.505626	0.484417
H	2.094547	-0.821295	2.142898
C	1.573020	1.143518	1.454956
H	2.558284	1.616600	1.518428
H	1.106870	1.302229	2.436367
C	0.764858	1.993804	0.475584
C	-1.334530	0.089072	2.010101
H	-0.704760	0.575812	2.762269
H	-2.273308	-0.135832	2.534435
O	1.153212	3.112637	0.190830
C	-0.270360	0.385224	-1.153484
C	0.180353	-1.580389	-3.109710
C	-0.520437	0.643487	-2.507114
C	0.227137	-0.875353	-0.773860
C	0.441540	-1.841693	-1.764383

C	-0.300957	-0.327589	-3.484020
H	-0.895070	1.622214	-2.797194
H	0.821887	-2.818536	-1.472677
H	-0.504818	-0.104094	-4.527770
H	0.355803	-2.349656	-3.857057

9,10-benzobicyclo[3.3.2]decane

C	-0.057010	-1.507965	-0.333576
C	-0.057010	1.507965	-0.333576
C	-1.347547	1.298293	-1.168042
C	-1.442594	0.000000	-1.977273
C	-1.347547	-1.298293	-1.168042
H	-2.209957	1.374570	-0.491598
H	-1.429726	2.140316	-1.869889
H	-0.665203	-0.000000	-2.752931
H	-2.396641	0.000000	-2.521463
H	-2.209957	-1.374570	-0.491598
C	1.249722	1.313893	-1.167923
H	1.015047	1.429850	-2.234791
H	1.938708	2.132957	-0.925441
C	1.249722	-1.313893	-1.167923
H	1.015047	-1.429850	-2.234791
C	2.017689	-0.000000	-0.943035
H	2.896773	0.000000	-1.601262
H	-1.429726	-2.140316	-1.869889
H	1.938708	-2.132957	-0.925441
H	-0.083127	-2.563734	-0.036206
H	-0.083127	2.563734	-0.036206
C	-0.066075	0.706999	0.962669
C	-0.113486	-0.696224	3.404380
C	-0.086679	1.382058	2.188626
C	-0.066075	-0.706999	0.962669
C	-0.086679	-1.382058	2.188626
C	-0.113486	0.696224	3.404380
H	-0.084921	2.470365	2.188674
H	-0.084921	-2.470365	2.188674
H	-0.134179	1.248743	4.340229
H	-0.134179	-1.248743	4.340229
H	2.408434	0.000000	0.081738

1-Azabicyclo[4.3.1]decane-10-one 32a (Table 6)

1-Azabicyclo[4.3.1]decane

H	1.924320	-1.003058	-1.041915
C	1.235522	-0.348127	-0.488329
C	0.935527	2.205764	-0.448637
N	-1.025944	0.653966	-0.576545
C	-0.490163	1.886493	0.027657
C	-0.021220	-0.095956	-1.332999
C	1.915657	1.029192	-0.222999
H	-1.151513	2.739854	-0.190051
H	0.237600	0.461971	-2.242168
H	1.289936	3.102181	0.073994
H	-0.473530	1.793576	1.129028
H	-0.460389	-1.029344	-1.688521
H	2.785142	1.160917	-0.878651
C	-0.237439	-2.135309	0.732302
H	0.101098	-2.914871	0.036666
H	-0.304899	-2.622777	1.712755
C	0.841514	-1.040829	0.836932
H	0.490408	-0.277720	1.543452
H	1.742797	-1.470509	1.295029
C	-1.661675	-1.651969	0.312187
H	-1.919783	-2.042514	-0.678843
H	-2.407683	-2.082697	0.992353
H	0.908179	2.467929	-1.513059
H	2.300921	1.057748	0.804863
C	-1.881588	-0.129513	0.331616
H	-1.729834	0.222017	1.366472
H	-2.942962	0.063585	0.107412

1-Azabicyclo[4.3.1]decan-10-one

H	0.472247	2.208698	-0.962325
C	0.003241	1.389044	-0.410387
C	-2.378590	0.566986	-0.067943
N	-0.552004	-0.971308	-0.664332
C	-1.678746	-0.756261	0.253410
C	-1.422598	1.769872	0.066046
H	-2.382857	-1.591526	0.140130
H	-1.808163	2.608408	-0.524328
H	-3.252914	0.686055	0.581689
H	-1.354367	-0.763325	1.307370
H	-1.379667	2.113683	1.107728
C	2.121706	0.032581	0.492690
H	2.849544	0.591237	-0.108365
H	2.605081	-0.137969	1.462793
C	0.909585	0.955558	0.788507
H	0.278364	0.467874	1.539793
H	1.290498	1.865750	1.270428
C	0.476505	-1.946454	-0.234708
H	0.475572	-2.836391	-0.877238
H	0.190007	-2.280857	0.771025
C	1.903537	-1.353718	-0.208861
H	2.549797	-2.097529	0.273292
H	2.247433	-1.277795	-1.242122
C	-0.008728	0.160380	-1.301849
O	0.599050	0.084538	-2.354094
H	-2.753536	0.512469	-1.098350

Bicyclo[4.3.1]decan-10-one

H	0.555209	2.176358	-0.992234
C	0.300488	1.320268	-0.359058
C	-2.225374	0.918273	-0.465271
C	-2.064297	-0.617572	-0.571708
C	-1.078605	1.575198	0.322250
H	-2.661490	-0.983529	-1.413794
H	-3.190777	1.158055	-0.003994
H	-2.467104	-1.098964	0.329039
H	-1.251932	2.654079	0.412026
C	2.308182	-0.191122	0.385584
H	2.647175	-0.169137	-0.656194
H	3.219578	-0.148566	0.994403
C	1.478875	1.080808	0.654691
H	1.081378	1.051051	1.677425
H	2.151545	1.944863	0.616528
C	1.582307	-1.535979	0.676856
H	1.972654	-2.304856	-0.002653
H	1.843021	-1.870771	1.689675
H	-2.251416	1.350940	-1.475043
H	-1.073740	1.183124	1.347012
C	0.044825	-1.504607	0.599240
H	-0.332104	-0.856117	1.398385
H	-0.345570	-2.504551	0.829486
C	-0.572097	-1.053878	-0.749420
H	-0.494846	-1.866603	-1.478910
C	0.183465	0.136026	-1.317972

O	0.640649	0.157207	-2.446350

Bicyclo[4.3.1]decane

H	0.613179	2.159391	-0.950005
C	0.317999	1.288489	-0.350559
C	-2.239926	0.919685	-0.430751
C	-2.077314	-0.618400	-0.487866
C	0.180942	0.104008	-1.332103
C	-1.070336	1.603395	0.296440
H	-2.703490	-1.011270	-1.298812
H	-0.346649	0.436211	-2.235334
H	-3.185804	1.174514	0.063374
H	-2.466372	-1.064235	0.437815
H	1.165686	-0.228710	-1.673820
H	-1.235668	2.687541	0.331271
C	2.318979	-0.180391	0.551035
H	2.838922	-0.116723	-0.412610
H	3.114229	-0.136957	1.306649
C	1.433837	1.066952	0.729952
H	0.975806	1.027385	1.726768
H	2.092730	1.944802	0.751080
C	1.587868	-1.552993	0.671886
H	1.948306	-2.228808	-0.115788
H	1.878353	-2.024202	1.619654
H	-2.317299	1.321201	-1.449577
H	-1.073202	1.268425	1.342272
C	0.048836	-1.509163	0.640468
H	-0.298503	-0.855738	1.450455
H	-0.336924	-2.507171	0.891136
C	-0.595434	-1.055994	-0.691925
H	-0.568751	-1.911244	-1.381107

B3LYP/6-31G(d,p) vibrational frequencies of lactams 3a-c, 4a, 5a, penicillin models 14_{eq} and 15_{eq}, and bicyclic amino acids 20_{eq} and 21_{eq}.

β-Propiolactam **3a**:

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	114.312	0.6837	1.2395	13.3650	8.1067	42.40	15.98
2	386.255	2.3103	0.8479	4.2449	6.2740	84.49	103.37
3	469.287	2.8070	0.6507	3.0942	5.5152	89.61	3.28
4	557.565	3.3350	0.4854	2.2121	4.6992	93.22	31.07
5	748.221	4.4754	0.2487	1.0620	3.0954	97.30	2.12
6	833.718	4.9867	0.1817	0.7596	2.4968	98.21	0.06
7	882.926	5.2811	0.1512	0.6252	2.1914	98.59	2.45
8	971.063	5.8082	0.1081	0.4397	1.7154	99.08	15.29
9	1015.706	6.0753	0.0910	0.3673	1.5076	99.26	2.59
10	1055.461	6.3131	0.0780	0.3127	1.3402	99.39	0.89
11	1158.850	6.9315	0.0519	0.2050	0.9762	99.63	0.20
12	1178.067	7.0464	0.0480	0.1894	0.9189	99.66	86.57
13	1192.857	7.1349	0.0453	0.1782	0.8768	99.68	0.05
14	1203.865	7.2007	0.0433	0.1703	0.8466	99.70	0.54
15	1307.621	7.8213	0.0285	0.1107	0.6040	99.82	28.27
16	1406.054	8.4101	0.0190	0.0732	0.4337	99.89	34.28
17	1475.694	8.8266	0.0143	0.0546	0.3411	99.92	4.49
18	1544.723	9.2395	0.0107	0.0407	0.2678	99.94	7.15
19	1899.128	11.3593	0.0024	0.0088	0.0731	99.99	522.04
20	3052.899	18.2604	0.0000	0.0001	0.0007	100.00	58.78
21	3098.254	18.5317	0.0000	0.0000	0.0006	100.00	32.15
22	3101.486	18.5510	0.0000	0.0000	0.0006	100.00	8.64
23	3160.574	18.9044	0.0000	0.0000	0.0005	100.00	11.38
24	3618.198	21.6416	0.0000	0.0000	0.0001	100.00	19.67
Total Vibrations		211.9351	4.3456	27.5138	42.2827	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	161.9221	12.4716		
Rotation			3.7184	103.6762	12.4716		
Totals			226.1964	293.1122	67.2259		

Vibrational(v) Corrections:

Temp. Correction Hv	226.1964
Entropy Correction (Hv-TSv)	138.8051

N-Methyl-β-propiolactam **3b**:

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 4 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	121.006	0.7238	1.2395	12.9044	8.0821	44.23	3.53
2*	146.351	0.8754	1.2395	11.3767	7.9773	50.65	3.19
3*	195.285	1.1681	1.2395	9.1087	7.7255	61.03	1.09
4*	248.380	1.4856	1.2395	7.2886	7.3866	69.84	5.68
5	477.166	2.8541	0.6342	3.0030	5.4421	90.00	2.25
6	551.220	3.2970	0.4959	2.2662	4.7572	93.01	3.84
7	716.699	4.2868	0.2786	1.2004	3.3370	96.85	0.82
8	775.333	4.6375	0.2253	0.9553	2.8964	97.63	1.70
9	833.125	4.9832	0.1821	0.7614	2.5007	98.21	1.19
10	948.678	5.6744	0.1178	0.4810	1.8279	98.97	0.57
11	988.557	5.9129	0.1011	0.4098	1.6314	99.15	23.03
12	1050.009	6.2804	0.0796	0.3197	1.3622	99.37	3.32
13	1084.190	6.4849	0.0697	0.2782	1.2291	99.47	61.73
14	1126.622	6.7387	0.0589	0.2339	1.0793	99.56	0.08
15	1176.226	7.0354	0.0484	0.1908	0.9243	99.66	3.14
16	1188.204	7.1070	0.0461	0.1816	0.8899	99.68	0.02
17	1200.629	7.1814	0.0439	0.1726	0.8554	99.70	1.20
18	1265.069	7.5668	0.0339	0.1321	0.6947	99.78	15.85
19	1309.311	7.8314	0.0283	0.1099	0.6006	99.82	24.29
20	1429.207	8.5486	0.0173	0.0664	0.4006	99.90	107.47
21	1454.176	8.6979	0.0156	0.0598	0.3676	99.91	18.08
22	1481.024	8.8585	0.0140	0.0534	0.3349	99.92	0.37
23	1494.810	8.9409	0.0132	0.0503	0.3191	99.93	8.08
24	1526.466	9.1303	0.0116	0.0440	0.2856	99.94	11.94
25	1547.736	9.2575	0.0106	0.0402	0.2649	99.94	6.09
26	1876.605	11.2246	0.0026	0.0098	0.0796	99.99	501.88
27	3021.925	18.0751	0.0000	0.0001	0.0008	100.00	53.97
28	3037.611	18.1689	0.0000	0.0001	0.0008	100.00	64.77
29	3074.950	18.3923	0.0000	0.0000	0.0007	100.00	48.27
30	3080.430	18.4251	0.0000	0.0000	0.0006	100.00	23.11
31	3098.344	18.5322	0.0000	0.0000	0.0006	100.00	12.49
32	3140.346	18.7834	0.0000	0.0000	0.0005	100.00	5.00
33	3156.053	18.8774	0.0000	0.0000	0.0005	100.00	11.63
Total Vibrations		286.0375	7.4866	51.6988	63.2564	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	164.1684	12.4716		
Rotation			3.7184	110.0015	12.4716		
Totals			303.4399	325.8686	88.1996		

Vibrational(v) Corrections:

Temp. Correction Hv	303.4399
Entropy Correction (Hv-TSv)	206.2821

γ-Butyrolactam **4a**:

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 2 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	141.367	0.8456	1.2395	11.6535	7.9993	49.45	0.88
2*	192.030	1.1486	1.2395	9.2388	7.7441	60.41	4.41
3	465.736	2.7857	0.6582	3.1362	5.5482	89.43	10.49
4	492.462	2.9456	0.6032	2.8335	5.3000	90.71	65.29
5	568.732	3.4018	0.4674	2.1199	4.5977	93.57	43.03
6	635.767	3.8027	0.3710	1.6404	4.0040	95.35	23.19
7	694.469	4.1538	0.3017	1.3083	3.5139	96.50	7.68
8	815.088	4.8753	0.1947	0.8174	2.6199	98.04	5.63
9	889.637	5.3212	0.1474	0.6088	2.1520	98.63	3.59
10	911.815	5.4539	0.1356	0.5574	2.0255	98.77	1.86
11	922.193	5.5159	0.1303	0.5348	1.9683	98.83	0.80
12	1004.708	6.0095	0.0950	0.3840	1.5568	99.22	9.84
13	1080.277	6.4615	0.0707	0.2827	1.2438	99.46	16.01
14	1095.778	6.5542	0.0666	0.2654	1.1866	99.49	0.64
15	1190.558	7.1211	0.0457	0.1799	0.8833	99.68	4.11
16	1214.807	7.2662	0.0415	0.1627	0.8175	99.72	1.10
17	1247.366	7.4609	0.0364	0.1422	0.7360	99.76	17.17
18	1269.809	7.5951	0.0332	0.1295	0.6841	99.78	72.80
19	1308.031	7.8238	0.0284	0.1105	0.6031	99.82	23.93
20	1343.744	8.0374	0.0246	0.0952	0.5355	99.85	17.62
21	1373.241	8.2138	0.0218	0.0841	0.4848	99.87	10.53
22	1454.959	8.7026	0.0156	0.0596	0.3666	99.91	41.37
23	1485.771	8.8869	0.0137	0.0523	0.3294	99.92	3.00
24	1510.945	9.0375	0.0123	0.0470	0.3016	99.93	5.80
25	1550.867	9.2762	0.0104	0.0397	0.2620	99.94	4.13
26	1834.239	10.9712	0.0031	0.0117	0.0933	99.99	414.31
27	3004.375	17.9702	0.0000	0.0001	0.0009	100.00	68.04
28	3061.649	18.3127	0.0000	0.0001	0.0007	100.00	13.78
29	3071.552	18.3720	0.0000	0.0000	0.0007	100.00	12.58
30	3085.179	18.4535	0.0000	0.0000	0.0006	100.00	49.28
31	3125.456	18.6944	0.0000	0.0000	0.0005	100.00	17.96
32	3136.586	18.7609	0.0000	0.0000	0.0005	100.00	19.72
33	3643.441	21.7926	0.0000	0.0000	0.0001	100.00	28.04
Total Vibrations		292.0241	6.0074	36.4958	57.5610	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	164.1684	12.4716		
Rotation			3.7184	109.1273	12.4716		
Totals			307.9473	309.7914	82.5043		

Vibrational(v) Corrections:

Temp. Correction	Hv	307.9473
Entropy Correction	(Hv-TSv)	215.5830

δ-Valerolactam **5a:**

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 2 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	107.116	0.6407	1.2395	13.8929	8.1317	40.36	0.70
2*	162.815	0.9738	1.2395	10.5303	7.8996	54.42	2.25
3	324.620	1.9417	1.0246	5.3836	6.8040	79.12	1.79
4	422.357	2.5263	0.7568	3.6986	5.9480	86.97	7.59
5	444.704	2.6599	0.7045	3.3972	5.7428	88.31	7.15
6	491.432	2.9394	0.6052	2.8446	5.3096	90.67	6.67
7	536.126	3.2067	0.5217	2.4002	4.8958	92.48	20.27
8	662.966	3.9654	0.3373	1.4775	3.7729	95.92	47.22
9	666.410	3.9860	0.3332	1.4580	3.7442	95.99	40.76
10	771.854	4.6167	0.2282	0.9684	2.9214	97.59	2.59
11	840.526	5.0275	0.1772	0.7395	2.4529	98.27	4.82
12	873.548	5.2250	0.1566	0.6489	2.2474	98.52	0.08
13	938.645	5.6143	0.1224	0.5007	1.8801	98.92	4.80
14	947.622	5.6680	0.1183	0.4831	1.8333	98.97	6.83
15	1007.926	6.0287	0.0938	0.3791	1.5422	99.23	4.61
16	1066.557	6.3794	0.0747	0.2989	1.2963	99.42	3.89
17	1111.606	6.6489	0.0625	0.2488	1.1304	99.53	5.28
18	1124.059	6.7234	0.0595	0.2364	1.0879	99.56	13.93
19	1183.442	7.0786	0.0470	0.1852	0.9034	99.67	27.14
20	1203.916	7.2010	0.0433	0.1702	0.8465	99.70	4.90
21	1280.615	7.6598	0.0318	0.1239	0.6602	99.79	3.63
22	1298.452	7.7665	0.0296	0.1150	0.6226	99.81	2.99
23	1326.262	7.9328	0.0264	0.1024	0.5677	99.83	65.87
24	1365.998	8.1705	0.0224	0.0867	0.4968	99.86	19.88
25	1384.782	8.2828	0.0208	0.0801	0.4662	99.87	49.71
26	1392.610	8.3297	0.0201	0.0775	0.4540	99.88	6.88
27	1407.136	8.4165	0.0189	0.0729	0.4321	99.89	12.76
28	1475.205	8.8237	0.0143	0.0547	0.3417	99.92	16.77
29	1495.388	8.9444	0.0131	0.0502	0.3185	99.93	24.58
30	1505.121	9.0026	0.0126	0.0482	0.3078	99.93	5.81
31	1516.680	9.0718	0.0120	0.0459	0.2956	99.93	14.70
32	1541.211	9.2185	0.0109	0.0413	0.2711	99.94	9.66
33	1791.002	10.7126	0.0038	0.0141	0.1096	99.98	356.13
34	2990.191	17.8853	0.0000	0.0001	0.0009	100.00	60.06
35	3036.014	18.1594	0.0000	0.0001	0.0008	100.00	17.59
36	3043.629	18.2049	0.0000	0.0001	0.0007	100.00	11.24
37	3046.151	18.2200	0.0000	0.0001	0.0007	100.00	21.59
38	3067.498	18.3477	0.0000	0.0000	0.0007	100.00	50.14
39	3086.390	18.4607	0.0000	0.0000	0.0006	100.00	38.07
40	3096.264	18.5198	0.0000	0.0000	0.0006	100.00	42.84
41	3117.334	18.6458	0.0000	0.0000	0.0006	100.00	13.85
42	3600.725	21.5371	0.0000	0.0000	0.0001	100.00	18.22
Total Vibrations		369.3643	8.1828	50.8554	75.7403	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	166.0711	12.4716		
Rotation			3.7184	113.8355	12.4716		
Totals			387.4629	330.7620	100.6835		

Vibrational(v) Corrections:

Temp. Correction Hv	387.4629
Entropy Correction (Hv-TSv)	288.8462

N-Acetyl-β-propiolactam **3c**:

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 5 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	80.919	0.4840	1.2395	16.1855	8.2096	32.33	7.25
2*	111.588	0.6674	1.2395	13.5607	8.1164	41.64	4.02
3*	129.963	0.7774	1.2395	12.3284	8.0472	46.59	0.54
4*	171.249	1.0243	1.2395	10.1324	7.8570	56.24	13.86
5*	207.803	1.2429	1.2395	8.6310	7.6513	63.31	0.08
6	370.795	2.2178	0.8897	4.5040	6.4106	83.29	2.25
7	387.096	2.3153	0.8457	4.2313	6.2665	84.56	2.06
8	532.663	3.1860	0.5278	2.4321	4.9277	92.35	0.85
9	592.917	3.5464	0.4303	1.9330	4.3800	94.28	18.66
10	597.926	3.5764	0.4230	1.8963	4.3354	94.42	8.59
11	672.644	4.0233	0.3259	1.4234	3.6923	96.11	3.94
12	772.976	4.6234	0.2273	0.9642	2.9133	97.60	3.60
13	812.300	4.8586	0.1967	0.8264	2.6387	98.02	2.39
14	932.367	5.5768	0.1254	0.5135	1.9134	98.89	8.67
15	968.189	5.7911	0.1093	0.4448	1.7295	99.06	29.70
16	1041.036	6.2268	0.0825	0.3315	1.3991	99.34	53.58
17	1053.694	6.3025	0.0785	0.3150	1.3473	99.38	8.35
18	1061.499	6.3492	0.0762	0.3051	1.3162	99.40	2.55
19	1135.348	6.7909	0.0569	0.2257	1.0505	99.58	3.08
20	1155.722	6.9128	0.0525	0.2076	0.9859	99.62	1.20
21	1182.482	7.0728	0.0472	0.1860	0.9062	99.67	32.47
22	1193.182	7.1368	0.0452	0.1779	0.8759	99.68	0.04
23	1236.201	7.3941	0.0380	0.1489	0.7631	99.74	30.04
24	1333.291	7.9749	0.0257	0.0994	0.5545	99.84	30.54
25	1372.057	8.2067	0.0219	0.0845	0.4868	99.87	458.16
26	1416.547	8.4728	0.0182	0.0701	0.4184	99.89	129.01
27	1467.826	8.7795	0.0147	0.0564	0.3506	99.92	6.33
28	1473.756	8.8150	0.0144	0.0550	0.3434	99.92	0.08
29	1487.691	8.8984	0.0136	0.0519	0.3272	99.92	8.64
30	1532.324	9.1653	0.0113	0.0429	0.2798	99.94	3.97
31	1797.764	10.7530	0.0037	0.0137	0.1069	99.98	259.14
32	1882.154	11.2578	0.0026	0.0095	0.0779	99.99	379.16
33	3065.774	18.3374	0.0000	0.0000	0.0007	100.00	0.41
34	3089.438	18.4789	0.0000	0.0000	0.0006	100.00	23.81
35	3101.185	18.5492	0.0000	0.0000	0.0006	100.00	6.43
36	3132.904	18.7389	0.0000	0.0000	0.0005	100.00	3.07
37	3142.047	18.7936	0.0000	0.0000	0.0005	100.00	8.10
38	3159.611	18.8987	0.0000	0.0000	0.0005	100.00	10.99
39	3178.985	19.0145	0.0000	0.0000	0.0004	100.00	7.35
Total Vibrations		311.2319	10.9016	82.3885	90.6822	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	167.7168	12.4716		
Rotation			3.7184	117.6330	12.4716		
Totals			332.0493	367.7383	115.6255		

Vibrational(v) Corrections:

Temp. Correction Hv	332.0493
Entropy Correction (Hv-TSv)	222.4081

Penicillin model $\mathbf{15}_{eq}$ (HB):

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 13 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	36.621	0.2190	1.2395	22.7355	8.2928	16.20	3.26
2*	44.247	0.2647	1.2395	21.1678	8.2829	19.23	1.09
3*	56.461	0.3377	1.2395	19.1508	8.2632	23.85	3.10
4*	66.709	0.3990	1.2395	17.7742	8.2430	27.52	2.80
5*	69.644	0.4166	1.2395	17.4195	8.2366	28.54	1.24
6*	76.670	0.4586	1.2395	16.6286	8.2202	30.93	5.32
7*	128.315	0.7675	1.2395	12.4312	8.0538	46.16	8.76
8*	134.626	0.8052	1.2395	12.0451	8.0280	47.78	5.38
9*	167.860	1.0040	1.2395	10.2896	7.8743	55.52	6.02
10*	200.871	1.2015	1.2395	8.8914	7.6929	62.07	7.33
11*	223.007	1.3339	1.2395	8.0940	7.5564	65.91	3.28
12*	237.464	1.4203	1.2395	7.6223	7.4613	68.21	1.15
13*	252.058	1.5076	1.2395	7.1802	7.3609	70.37	0.04
14	263.172	1.5741	1.2294	6.8643	7.2816	71.92	1.57
15	301.741	1.8048	1.0974	5.8878	6.9889	76.69	0.44
16	303.027	1.8125	1.0932	5.8581	6.9787	76.83	1.69
17	335.798	2.0085	0.9905	5.1548	6.7111	80.22	7.00
18	356.726	2.1337	0.9292	4.7544	6.5330	82.12	3.36
19	378.923	2.2665	0.8675	4.3658	6.3390	83.94	0.46
20	434.981	2.6018	0.7269	3.5251	5.8323	87.74	30.62
21	461.180	2.7585	0.6680	3.1910	5.5904	89.20	36.54
22	465.997	2.7873	0.6577	3.1331	5.5458	89.45	37.42
23	510.327	3.0524	0.5686	2.6476	5.1342	91.48	26.54
24	524.146	3.1351	0.5431	2.5121	5.0063	92.03	3.87
25	575.649	3.4431	0.4565	2.0647	4.5351	93.78	5.13
26	591.130	3.5357	0.4330	1.9462	4.3960	94.23	17.05
27	620.559	3.7118	0.3912	1.7389	4.1359	94.99	0.76
28	623.328	3.7283	0.3874	1.7206	4.1117	95.06	17.01
29	635.428	3.8007	0.3714	1.6425	4.0069	95.34	15.49
30	683.206	4.0865	0.3140	1.3665	3.6054	96.30	6.71
31	713.318	4.2666	0.2820	1.2162	3.3636	96.80	49.73
32	731.568	4.3757	0.2641	1.1331	3.2217	97.07	2.76
33	750.000	4.4860	0.2471	1.0546	3.0821	97.32	4.02
34	805.701	4.8192	0.2016	0.8481	2.6835	97.95	2.33
35	847.796	5.0709	0.1724	0.7186	2.4065	98.33	4.27
36	882.524	5.2787	0.1514	0.6262	2.1938	98.59	16.85
37	925.900	5.5381	0.1285	0.5269	1.9481	98.85	7.55
38	939.529	5.6196	0.1220	0.4990	1.8755	98.93	21.91
39	954.363	5.7084	0.1153	0.4702	1.7988	99.00	2.13
40	966.363	5.7801	0.1101	0.4481	1.7385	99.06	0.60
41	989.861	5.9207	0.1006	0.4077	1.6252	99.16	4.00
42	1016.572	6.0804	0.0907	0.3661	1.5038	99.26	4.40
43	1028.980	6.1547	0.0864	0.3481	1.4499	99.30	15.32
44	1041.193	6.2277	0.0824	0.3313	1.3984	99.34	17.86
45	1056.683	6.3204	0.0776	0.3112	1.3353	99.39	5.55
46	1062.065	6.3526	0.0760	0.3044	1.3140	99.41	82.78
47	1157.092	6.9209	0.0522	0.2064	0.9816	99.62	15.96
48	1180.804	7.0628	0.0475	0.1873	0.9110	99.66	131.01
49	1189.329	7.1138	0.0459	0.1808	0.8867	99.68	2.25
50	1200.480	7.1805	0.0439	0.1727	0.8558	99.70	16.58
51	1218.968	7.2910	0.0408	0.1600	0.8066	99.72	44.19
52	1227.882	7.3444	0.0393	0.1542	0.7838	99.73	7.84
53	1232.410	7.3714	0.0386	0.1513	0.7725	99.74	35.31
54	1258.953	7.5302	0.0347	0.1355	0.7087	99.77	134.16
55	1273.451	7.6169	0.0327	0.1276	0.6759	99.79	34.51
56	1290.732	7.7203	0.0305	0.1187	0.6386	99.80	27.28
57	1304.048	7.7999	0.0289	0.1123	0.6112	99.82	114.79
58	1348.378	8.0651	0.0241	0.0933	0.5272	99.85	39.49
59	1351.948	8.0864	0.0238	0.0919	0.5209	99.85	20.16
60	1385.242	8.2856	0.0207	0.0799	0.4655	99.88	441.38
61	1409.631	8.4315	0.0188	0.0722	0.4284	99.89	37.13
62	1416.492	8.4725	0.0182	0.0701	0.4185	99.89	12.94
63	1438.319	8.6031	0.0167	0.0639	0.3882	99.90	7.46
64	1480.902	8.8578	0.0140	0.0534	0.3350	99.92	22.23
65	1492.364	8.9263	0.0133	0.0509	0.3219	99.93	0.57
66	1500.790	8.9767	0.0129	0.0491	0.3125	99.93	8.58
67	1508.870	9.0250	0.0124	0.0474	0.3038	99.93	3.23
68	1515.038	9.0619	0.0121	0.0462	0.2973	99.93	6.08
69	1529.113	9.1461	0.0114	0.0435	0.2829	99.94	10.64
70	1541.959	9.2230	0.0108	0.0412	0.2704	99.94	355.89
71	1795.322	10.7384	0.0037	0.0139	0.1078	99.98	256.12
72	1859.542	11.1225	0.0028	0.0105	0.0849	99.99	278.23
73	1900.692	11.3687	0.0024	0.0088	0.0727	99.99	328.98
74	3053.423	18.2635	0.0000	0.0001	0.0007	100.00	15.13
75	3057.882	18.2902	0.0000	0.0001	0.0007	100.00	7.08
76	3059.553	18.3002	0.0000	0.0001	0.0007	100.00	3.85
77	3077.848	18.4096	0.0000	0.0000	0.0007	100.00	4.60
78	3106.506	18.5810	0.0000	0.0000	0.0006	100.00	30.30
79	3121.617	18.6714	0.0000	0.0000	0.0005	100.00	10.52
80	3129.492	18.7185	0.0000	0.0000	0.0005	100.00	9.43
81	3129.974	18.7214	0.0000	0.0000	0.0005	100.00	19.04
82	3132.289	18.7352	0.0000	0.0000	0.0005	100.00	14.19
83	3138.318	18.7713	0.0000	0.0000	0.0005	100.00	3.17
84	3145.503	18.8143	0.0000	0.0000	0.0005	100.00	10.85
85	3167.414	18.9453	0.0000	0.0000	0.0004	100.00	6.09
86	3637.582	21.7576	0.0000	0.0000	0.0001	100.00	20.81
87	3638.666	21.7641	0.0000	0.0000	0.0001	100.00	171.42
Total Vibrations		640.4632	30.7998	251.9572	243.0148	-Unscaled-	

Ideal Gas	2.4789		
Translation	3.7184	178.0145	12.4716
Rotation	3.7184	138.7122	12.4716
Totals	681.1787	568.6839	267.9580

Vibrational(v) Corrections:	
Temp. Correction Hv	681.1787
Entropy Correction (Hv-TSv)	511.6256

Penicillin model **15**$_{eq}$ (HB):

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 13 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	i 62.919	0.0000	1.2395	0.0000	8.3144	0.00	0.15
2*	36.791	0.2201	1.2395	22.6970	8.2926	16.27	3.94
3*	39.433	0.2359	1.2395	22.1221	8.2894	17.33	1.33
4*	48.172	0.2881	1.2395	20.4641	8.2771	20.74	1.62
5*	60.742	0.3633	1.2395	18.5472	8.2551	25.41	0.18
6*	67.611	0.4044	1.2395	17.6636	8.2410	27.84	10.48
7*	119.110	0.7124	1.2395	13.0320	8.0892	43.72	2.54
8*	132.905	0.7950	1.2395	12.1484	8.0352	47.34	4.72
9*	158.086	0.9456	1.2395	10.7635	7.9226	53.37	2.59
10*	199.948	1.1960	1.2395	8.9268	7.6983	61.90	7.42
11*	223.402	1.3362	1.2395	8.0806	7.5539	65.98	2.14
12*	241.634	1.4453	1.2395	7.4927	7.4331	68.84	1.81
13*	251.500	1.5043	1.2395	7.1966	7.3648	70.29	0.07
14	262.877	1.5724	1.2304	6.8725	7.2837	71.88	0.63
15	301.641	1.8042	1.0977	5.8901	6.9897	76.67	0.67
16	311.457	1.8629	1.0660	5.6675	6.9113	77.75	0.32
17	329.722	1.9722	1.0090	5.2778	6.7618	79.63	0.99
18	357.449	2.1380	0.9271	4.7412	6.5268	82.18	0.75
19	382.696	2.2890	0.8574	4.3031	6.3056	84.23	0.88
20	426.385	2.5503	0.7471	3.6423	5.9112	87.22	16.10
21	454.490	2.7185	0.6827	3.2731	5.6524	88.84	52.10
22	461.477	2.7602	0.6674	3.1874	5.5877	89.21	12.74
23	511.903	3.0619	0.5657	2.6318	5.1196	91.54	34.82
24	524.881	3.1395	0.5417	2.5051	4.9995	92.06	11.65
25	566.474	3.3883	0.4710	2.1383	4.6182	93.50	19.50
26	587.147	3.5119	0.4389	1.9760	4.4316	94.12	9.63
27	611.904	3.6600	0.4031	1.7975	4.2117	94.78	76.75
28	621.027	3.7146	0.3905	1.7358	4.1318	95.01	7.32
29	629.348	3.7643	0.3794	1.6813	4.0594	95.20	4.20
30	674.908	4.0368	0.3233	1.4110	3.6736	96.15	55.40
31	686.143	4.1040	0.3107	1.3511	3.5814	96.35	12.73
32	731.718	4.3766	0.2640	1.1324	3.2205	97.07	21.57
33	752.133	4.4988	0.2452	1.0459	3.0661	97.35	26.97
34	807.762	4.8315	0.2000	0.8413	2.6695	97.97	4.94
35	849.762	5.0827	0.1712	0.7130	2.3941	98.34	7.83
36	877.420	5.2481	0.1543	0.6391	2.2242	98.55	17.72
37	923.905	5.5262	0.1295	0.5311	1.9590	98.84	4.95
38	940.219	5.6238	0.1217	0.4976	1.8718	98.93	15.60
39	953.253	5.7017	0.1158	0.4723	1.8044	98.99	1.70
40	962.107	5.7547	0.1119	0.4558	1.7597	99.04	0.44
41	989.096	5.9161	0.1009	0.4090	1.6288	99.15	1.87
42	1015.611	6.0747	0.0911	0.3675	1.5080	99.26	8.35
43	1035.709	6.1949	0.0842	0.3388	1.4213	99.32	9.00
44	1044.858	6.2496	0.0813	0.3264	1.3833	99.35	8.86
45	1056.000	6.3163	0.0778	0.3120	1.3381	99.39	7.82
46	1091.160	6.5266	0.0678	0.2704	1.2034	99.48	76.18
47	1161.127	6.9451	0.0514	0.2031	0.9693	99.63	24.32
48	1183.034	7.0761	0.0471	0.1855	0.9046	99.67	72.06
49	1195.958	7.1534	0.0447	0.1759	0.8682	99.69	11.97
50	1200.386	7.1799	0.0439	0.1727	0.8561	99.70	2.78
51	1201.537	7.1868	0.0437	0.1719	0.8529	99.70	194.17
52	1222.160	7.3101	0.0403	0.1579	0.7984	99.73	19.09
53	1245.070	7.4472	0.0367	0.1436	0.7415	99.75	19.89
54	1263.573	7.5578	0.0341	0.1329	0.6981	99.78	126.59
55	1275.963	7.6319	0.0324	0.1263	0.6704	99.79	39.10
56	1292.271	7.7295	0.0303	0.1180	0.6354	99.80	16.53
57	1322.595	7.9109	0.0268	0.1040	0.5747	99.83	221.64
58	1350.692	8.0789	0.0239	0.0924	0.5231	99.85	19.69
59	1371.549	8.2037	0.0219	0.0847	0.4876	99.87	19.41
60	1396.529	8.3531	0.0198	0.0762	0.4480	99.88	64.56
61	1408.044	8.4220	0.0189	0.0726	0.4307	99.89	37.55
62	1418.019	8.4816	0.0181	0.0696	0.4163	99.89	10.19
63	1439.671	8.6111	0.0166	0.0636	0.3864	99.90	6.32
64	1480.496	8.8553	0.0140	0.0535	0.3355	99.92	17.89
65	1494.844	8.9412	0.0132	0.0503	0.3191	99.93	0.87
66	1499.700	8.9702	0.0129	0.0493	0.3137	99.93	8.77
67	1507.085	9.0144	0.0125	0.0478	0.3057	99.93	2.93
68	1517.068	9.0741	0.0120	0.0458	0.2952	99.93	6.15
69	1527.232	9.1349	0.0115	0.0439	0.2848	99.94	9.21
70	1544.670	9.2392	0.0107	0.0407	0.2678	99.94	366.35
71	1793.564	10.7279	0.0037	0.0140	0.1085	99.98	266.84
72	1828.358	10.9360	0.0032	0.0120	0.0954	99.99	244.14
73	1888.822	11.2977	0.0025	0.0093	0.0760	99.99	380.19
74	3050.890	18.2484	0.0000	0.0001	0.0007	100.00	14.61
75	3054.385	18.2693	0.0000	0.0001	0.0007	100.00	12.08
76	3059.241	18.2983	0.0000	0.0001	0.0007	100.00	4.47
77	3074.665	18.3906	0.0000	0.0000	0.0007	100.00	5.82
78	3115.242	18.6333	0.0000	0.0000	0.0006	100.00	21.57
79	3121.132	18.6685	0.0000	0.0000	0.0005	100.00	16.73
80	3124.204	18.6869	0.0000	0.0000	0.0005	100.00	13.09
81	3129.050	18.7159	0.0000	0.0000	0.0005	100.00	10.55
82	3130.944	18.7272	0.0000	0.0000	0.0005	100.00	8.67
83	3134.667	18.7495	0.0000	0.0000	0.0005	100.00	12.52
84	3143.592	18.8029	0.0000	0.0000	0.0005	100.00	14.74
85	3164.554	18.9282	0.0000	0.0000	0.0005	100.00	7.21
86	3639.319	21.7680	0.0000	0.0000	0.0001	100.00	26.54
87	3743.649	22.3920	0.0000	0.0000	0.0000	100.00	69.44
Total Vibrations		640.1666	30.8859	240.0881	243.6465	-Unscaled-	

Ideal Gas	2.4789		
Translation	3.7184	178.0145	12.4716
Rotation	3.7184	138.7367	12.4716
Totals	680.9682	556.8393	268.5897

Vibrational(v) Corrections:

Temp. Correction	Hv	680.9682
Entropy Correction	(Hv-TSv)	514.9466

1-Aza-4-thiabicyclo[3.2.0]heptan-2-carboxylic acid HB **20**$_{eq}$

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 5 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	42.108	0.2519	1.2395	21.5782	8.2859	18.39	1.04
2*	75.280	0.4503	1.2395	16.7790	8.2236	30.46	0.59
3*	146.031	0.8735	1.2395	11.3942	7.9787	50.57	1.48
4*	154.423	0.9237	1.2395	10.9495	7.9401	52.54	1.05
5*	242.863	1.4526	1.2395	7.4550	7.4247	69.02	3.16
6	312.527	1.8693	1.0626	5.6438	6.9027	77.87	2.95
7	337.146	2.0166	0.9865	5.1279	6.6998	80.35	1.72
8	365.930	2.1887	0.9032	4.5890	6.4532	82.90	6.52
9	494.507	2.9578	0.5991	2.8116	5.2810	90.80	5.01
10	574.879	3.4385	0.4577	2.0708	4.5421	93.76	1.45
11	580.376	3.4714	0.4492	2.0278	4.4925	93.92	29.56
12	639.371	3.8243	0.3664	1.6178	3.9730	95.43	23.38
13	655.070	3.9182	0.3468	1.5231	3.8393	95.76	80.51
14	691.040	4.1333	0.3054	1.3258	3.5416	96.44	75.60
15	746.377	4.4643	0.2504	1.0696	3.1092	97.27	1.92
16	784.465	4.6921	0.2179	0.9218	2.8312	97.73	10.98
17	815.746	4.8792	0.1942	0.8153	2.6155	98.05	15.19
18	884.835	5.2925	0.1501	0.6205	2.1802	98.60	0.29
19	928.502	5.5537	0.1272	0.5215	1.9341	98.87	10.89
20	956.841	5.7232	0.1142	0.4656	1.7862	99.01	1.17
21	961.189	5.7492	0.1123	0.4575	1.7643	99.03	0.63
22	993.279	5.9411	0.0993	0.4021	1.6093	99.17	7.51
23	1019.736	6.0994	0.0896	0.3614	1.4899	99.27	10.22
24	1058.639	6.3321	0.0770	0.3087	1.3275	99.40	20.10
25	1088.747	6.5121	0.0684	0.2731	1.2122	99.48	36.12
26	1147.233	6.8620	0.0543	0.2150	1.0124	99.61	25.93
27	1155.847	6.9135	0.0525	0.2075	0.9855	99.62	141.46
28	1171.527	7.0073	0.0493	0.1945	0.9381	99.65	105.12
29	1200.016	7.1777	0.0440	0.1730	0.8571	99.69	20.71
30	1219.894	7.2966	0.0406	0.1593	0.8042	99.72	1.23
31	1245.950	7.4524	0.0366	0.1430	0.7393	99.76	43.91
32	1267.101	7.5789	0.0336	0.1310	0.6901	99.78	2.97
33	1270.340	7.5983	0.0331	0.1293	0.6829	99.78	1.55
34	1288.186	7.7051	0.0308	0.1200	0.6440	99.80	11.64
35	1318.619	7.8871	0.0272	0.1057	0.5823	99.83	4.04
36	1327.415	7.9397	0.0263	0.1019	0.5655	99.83	17.41
37	1358.915	8.1281	0.0231	0.0893	0.5088	99.86	4.58
38	1418.652	8.4854	0.0181	0.0695	0.4154	99.89	55.25
39	1497.354	8.9562	0.0130	0.0498	0.3163	99.93	1.63
40	1498.617	8.9637	0.0130	0.0495	0.3149	99.93	4.04
41	1537.448	9.1960	0.0110	0.0420	0.2747	99.94	3.30
42	1844.042	11.0298	0.0030	0.0112	0.0899	99.99	241.62
43	3029.257	18.1190	0.0000	0.0001	0.0008	100.00	42.81
44	3055.461	18.2757	0.0000	0.0001	0.0007	100.00	16.89
45	3083.298	18.4422	0.0000	0.0000	0.0006	100.00	22.85
46	3094.614	18.5099	0.0000	0.0000	0.0006	100.00	12.16
47	3094.834	18.5112	0.0000	0.0000	0.0006	100.00	17.44
48	3102.451	18.5568	0.0000	0.0000	0.0006	100.00	52.16
49	3154.174	18.8661	0.0000	0.0000	0.0005	100.00	3.63
50	3159.548	18.8983	0.0000	0.0000	0.0005	100.00	11.59
51	3746.954	22.4118	0.0000	0.0000	0.0000	100.00	51.24
Total Vibrations		399.7778	13.6845	103.1025	117.8641	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	171.9794	12.4716		
Rotation			3.7184	125.3114	12.4716		
Totals			423.3781	400.3934	142.8074		

Vibrational(v) Corrections:

Temp. Correction Hv	423.3781
Entropy Correction (Hv-TSv)	304.0008

1-Aza-4-thiabicyclo[3.2.0]heptan-2-carboxylic acid NHB **21**$_{eq}$

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

*Modifying values for 5 low frequency terms

	Term cm-1	ZPE kJ/mol	Enthalpy Correction kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1*	58.960	0.3527	1.2395	18.7931	8.2585	24.76	2.61
2*	93.190	0.5574	1.2395	15.0287	8.1757	36.22	1.67
3*	145.961	0.8730	1.2395	11.3980	7.9790	50.56	6.09
4*	178.254	1.0662	1.2395	9.8182	7.8202	57.69	5.93
5*	227.705	1.3620	1.2395	7.9368	7.5260	66.67	2.28
6	311.578	1.8636	1.0656	5.6648	6.9104	77.77	9.26
7	339.655	2.0316	0.9790	5.0783	6.6787	80.58	3.87
8	434.098	2.5965	0.7289	3.5370	5.8405	87.69	10.82
9	467.661	2.7972	0.6541	3.1134	5.5303	89.53	0.35
10	553.888	3.3130	0.4915	2.2433	4.7328	93.09	5.99
11	629.303	3.7641	0.3795	1.6816	4.0598	95.20	4.82
12	670.145	4.0084	0.3288	1.4372	3.7131	96.06	19.66
13	688.409	4.1176	0.3082	1.3393	3.5630	96.39	7.95
14	748.806	4.4789	0.2482	1.0595	3.0910	97.30	14.32
15	764.046	4.5700	0.2348	0.9984	2.9782	97.50	1.66
16	803.366	4.8052	0.2033	0.8560	2.6995	97.93	1.70
17	836.058	5.0007	0.1801	0.7526	2.4816	98.23	41.35
18	885.715	5.2977	0.1496	0.6184	2.1750	98.61	3.73
19	932.110	5.5753	0.1255	0.5140	1.9148	98.89	15.50
20	949.238	5.6777	0.1176	0.4800	1.8250	98.98	12.66
21	967.864	5.7891	0.1095	0.4454	1.7311	99.06	0.77
22	986.304	5.8994	0.1020	0.4136	1.6420	99.14	9.47
23	1021.704	6.1111	0.0889	0.3585	1.4813	99.28	9.82
24	1052.137	6.2932	0.0790	0.3169	1.3536	99.38	24.98
25	1081.132	6.4666	0.0705	0.2817	1.2406	99.46	14.83
26	1144.122	6.8434	0.0550	0.2177	1.0222	99.60	31.53
27	1157.835	6.9254	0.0521	0.2058	0.9794	99.63	8.17
28	1193.640	7.1396	0.0451	0.1776	0.8747	99.68	25.75
29	1222.740	7.3136	0.0402	0.1575	0.7969	99.73	2.31
30	1231.001	7.3630	0.0388	0.1522	0.7760	99.74	7.26
31	1239.659	7.4148	0.0375	0.1468	0.7546	99.75	11.02
32	1270.957	7.6020	0.0331	0.1289	0.6815	99.78	13.48
33	1273.232	7.6156	0.0328	0.1277	0.6764	99.79	10.17
34	1288.869	7.7091	0.0307	0.1197	0.6426	99.80	15.26
35	1317.801	7.8822	0.0273	0.1061	0.5839	99.83	5.69
36	1326.089	7.9318	0.0264	0.1024	0.5680	99.83	20.97
37	1357.223	8.1180	0.0233	0.0899	0.5118	99.86	4.58
38	1430.359	8.5554	0.0172	0.0661	0.3990	99.90	432.74
39	1494.848	8.9412	0.0132	0.0503	0.3191	99.93	4.26
40	1498.177	8.9611	0.0130	0.0496	0.3154	99.93	3.04
41	1534.199	9.1765	0.0112	0.0426	0.2779	99.94	6.50
42	1871.036	11.1913	0.0027	0.0100	0.0813	99.99	338.31
43	3052.162	18.2560	0.0000	0.0001	0.0007	100.00	36.93
44	3066.144	18.3396	0.0000	0.0000	0.0007	100.00	8.99
45	3084.175	18.4475	0.0000	0.0000	0.0006	100.00	15.13
46	3087.239	18.4658	0.0000	0.0000	0.0006	100.00	16.57
47	3099.778	18.5408	0.0000	0.0000	0.0006	100.00	25.06
48	3113.775	18.6245	0.0000	0.0000	0.0006	100.00	33.05
49	3161.349	18.9091	0.0000	0.0000	0.0005	100.00	10.29
50	3164.572	18.9283	0.0000	0.0000	0.0005	100.00	0.79
51	3457.197	20.6786	0.0000	0.0000	0.0001	100.00	299.90
Total Vibrations		400.5423	13.3416	96.1161	115.6669	-Unscaled-	
Ideal Gas			2.4789				
Translation			3.7184	171.9794	12.4716		
Rotation			3.7184	125.2225	12.4716		
Totals			423.7997	393.3180	140.6102		

Vibrational(v) Corrections:

Temp. Correction Hv	423.7997
Entropy Correction (Hv-TSv)	306.5319