Supplementary material for:

CONFORMATIONAL ANALYSIS AND FORMATION ENTHALPY FOR OF (3R,5S,6R)-6-ACETYLAMIDOPENICILLANIC ACID CALCULATED BY THE PM3, PM6 AND PM7 SEMIEMPIRICAL MO METHODS

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Table 1.

Hy-ID for conformers obtained by Conformational Search performed with HyperChem 7.5 softwares, standard formation enthalpy (Δ_fH^0), ν_0, , dihedral angles 5-1-2-3; 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
Hy-01	-145.0485	-9.867	-11.049	-3.146	-23.320	R	*syn*	26.62
Hy-02	-144.8221	-9.502	11.852	-3.016	22.384	S	*syn*	23.00
Hy-03	-144.5953	-10.698	-158.900	-2.503	22.936	S	*anti*	30.89
Hy-04	-144.5523	-9.508	-10.829	-2.954	-23.400	R	*syn*	26.72
Hy-05	-144.5207	-10.365	159.305	-3.143	-22.710	R	*anti*	26.42
Hy-06	-144.3950	-9.847	-13.048	-3.122	-23.340	R	*syn*	24.57
Hy-07	-144.3403	-9.178	12.022	-2.831	22.428	S	*syn*	22.75
Hy-08	-144.2523	-9.510	14.460	-3.143	22.400	S	*syn*	25.57
Hy-09	-144.0297	-10.362	-158.986	-2.411	23.052	S	*anti*	30.86
Hy-10	-143.8981	-10.129	159.131	-2.939	-22.607	R	*anti*	26.17
Hy-11	-143.9000	-9.471	-12.427	-2.868	-23.330	R	*syn*	24.52
Hy-12	-143.7653	-9.094	14.675	-3.019	22.480	S	*syn*	25.75
Hy-13	-142.2880	-10.650	-10.717	-1.572	-21.946	R	*syn*	33.67
Hy-14	-142.0939	-9.457	11.517	-4.072	26.330	S	*syn*	35.75
Hy-15	-141.9180	-11.447	12.953	-0.814	20.202	S	*syn*	35.22
Hy-16	-141.7140	-10.463	9.687	-1.781	22.667	S	*syn*	34.01
Hy-17	-141.6561	-10.517	-10.991	-1.302	-21.821	R	*syn*	33.87
Hy-18	-141.5746	-8.886	11.664	-3.975	26.342	S	*syn*	35.62
Hy-19	-141.2940	-11.251	12.798	-0.635	20.103	S	*syn*	35.41
Hy-20	-141.1377	-10.305	9.183	-1.613	22.833	S	*syn*	34.44
Hy-21	-140.9488	-11.485	-159.001	-1.379	23.313	S	*anti*	29.92
Hy-22	-140.8041	-11.266	158.962	-0.628	-23.075	R	*anti*	32.30
Hy-23	-140.6065	-10.598	159.580	-0.693	-23.132	R	*anti*	33.53
Hy-24	-140.5475	-10.624	164.316	-1.610	-23.386	R	*anti*	32.91
Hy-25	-140.5441	-10.790	-158.384	-0.961	22.988	S	*anti*	29.95
Hy-26	-140.3689	-10.458	164.354	-1.573	-23.320	R	*anti*	34.18
Hy-27	-139.7317	-10.318	160.907	-2.401	21.501	S	*anti*	32.98
Hy-28	-139.5458	-9.938	-161.057	-2.335	21.247	S	*anti*	34.34
Hy-29	-138.0281	-10.544	148.339	-3.344	32.691	S	*anti*	35.76
Hy-30	-137.3546	-9.719	148.703	-3.049	32.659	S	*anti*	34.38
Mean		**-10.208**		**-2.294**				**30.74**
SD		0.697		1.004				4.33

$$\Delta(\Delta_fH^0) = 7.6939 \text{kcal·mol}^{-1}$$

Table 2a.

PM3-Hy optimization-ID for distinct conformers obtained by OMEGA + PM3 softwares, standard formation enthalpy (Δ_fH^0), E_{HOMO}, E_{LUMO}, μ_{TOT}, ν_0, E_{ZVP}.

ID	Δ_fH^0 kcal·mol^{-1}	E_{HOMO} eV	E_{LUMO} eV	μ_{TOT} D	ν_0 cm^{-1}	E_{ZVP} kcal·mol^{-1}
Pn4-01/Pn4-02	-144.5208	-9.5191	-0.3086	1.466	26.48	149.658
Pn4-02/Pn4-03	-143.8980	-9.5570	-0.3366	2.629	26.21	149.642
Pn4-06 /Pn4-01	144.5954	-9.5077	-0.2828	1.437	30.86	149.640
Pn4-08/ Pn4-04	-144.0296	-9.5430	-0.3035	2.291	30.72	149.638
Pn4-09/Pn4-07	-140.6065	-9.4906	-0.2302	4.142	33.64	149.506
Pn4-13/Pn4-06	-140.8044	-9.4482	-0.1990	4.066	32.01	149.463
Pn4-23/Pn4-09	-140.5439	-9.5668	-0.3065	4.903	30.01	149.487
Pn4-24/Pn4-05	-140.9489	-9.5316	-0.2794	3.698	30.28	149.515
Pn4-33/Pn4-08	-140.5473	-9.3657	-0.1392	3.468	33.16	149.855

Pn4-01= Pn4-03 = Pn4-04 = Pn4-07 = Pn4-22 = Pn4-28 = Pn4-34 = Pn4-38 = Hy-05
Pn4-02= Pn4-05 = Pn4-14 = Pn4-20 = Pn4-27 = Pn4-29 = Pn4-37 = Hy-10
Pn4-06 = Pn4-02= Pn4-10 = Pn4-11 = Pn4-15 = Pn4-16= Pn4-21 = Hy-03
Pn4-08 = Pn4-12= Pn4-18 = Pn4-26 = Pn4-30 = Hy-09
Pn4-09 = Pn4-17= Pn4-32 = Hy-23
Pn4-13 = Pn4-19= Hy-22
Pn4-23 = Pn4-31= Hy-24
Pn4-24 = Pn4-25= Pn4-36 = Hy-21
Pn4-33 = Hy-25

Table 2b.

PM3-Hy optimization-ID in Δ_fH^0 order for distinct conformers obtained by OMEGA + PM3 softwares, standard formation enthalpy (Δ_fH^0), E_{HOMO}, E_{LUMO}, μ_{TOT}, ν_0, E_{ZVP},

ID	Δ_fH^0 kcal·mol^{-1}	E_{HOMO} eV	E_{LUMO} eV	μ_{TOT} D	ν_0 cm^{-1}	E_{ZVP} kcal·mol^{-1}
Pn4-01	144.5954	-9.5077	-0.2828	1.437	30.86	149.640
Pn4-02	-144.5208	-9.5191	-0.3086	1.466	26.48	149.658
Pn4-03	-143.8980	-9.5570	-0.3366	2.629	26.21	149.642
Pn4-04	-144.0296	-9.5430	-0.3035	2.291	30.72	149.638
Pn4-05	-140.9489	-9.5316	-0.2794	3.698	30.28	149.515
Pn4-06	-140.8044	-9.4482	-0.1990	4.066	32.01	149.463
Pn4-07	-140.6065	-9.4906	-0.2302	4.142	33.64	149.506
Pn4-08	-140.5473	-9.3657	-0.1392	3.468	33.16	149.855
Pn4-09	-140.5439	-9.5668	-0.3065	4.903	30.01	149.487

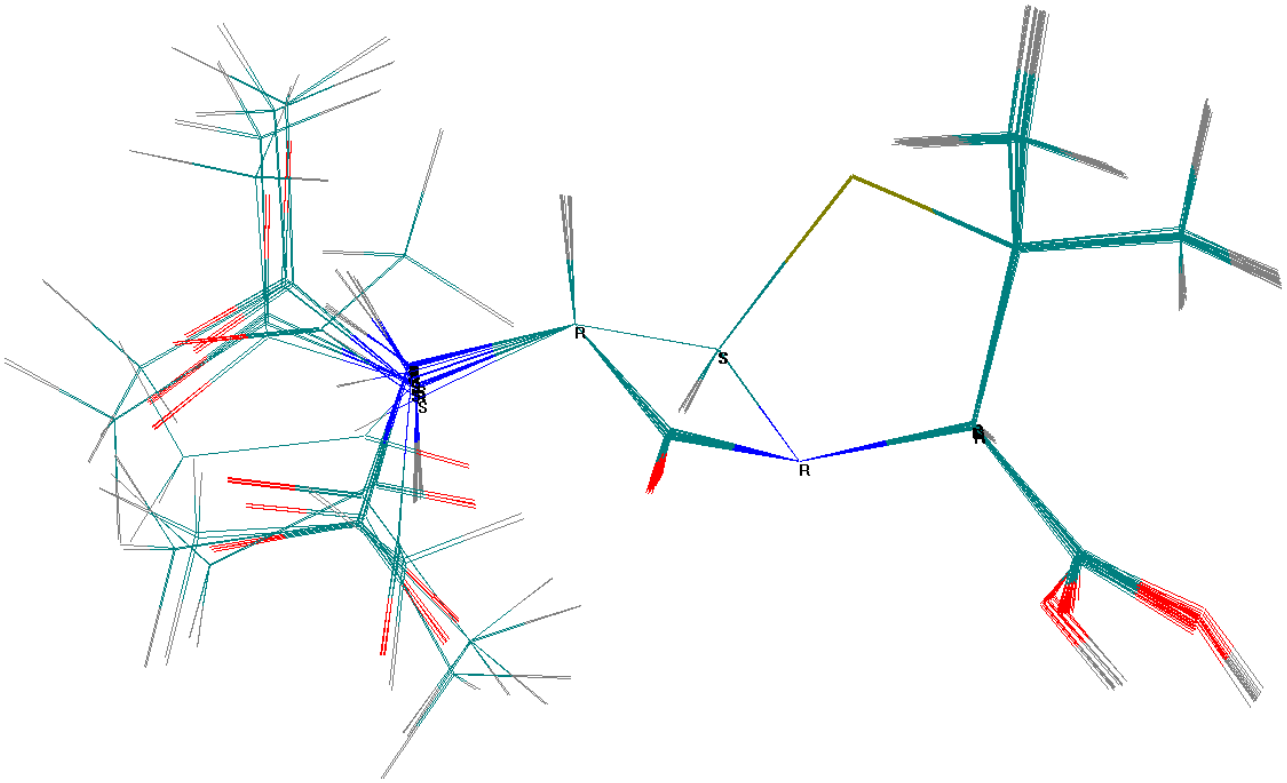


Fig. 1 a. Puckering of the thiazolidinic ring in PM3 HyperChem 7.5 (with the hydrogen atoms)

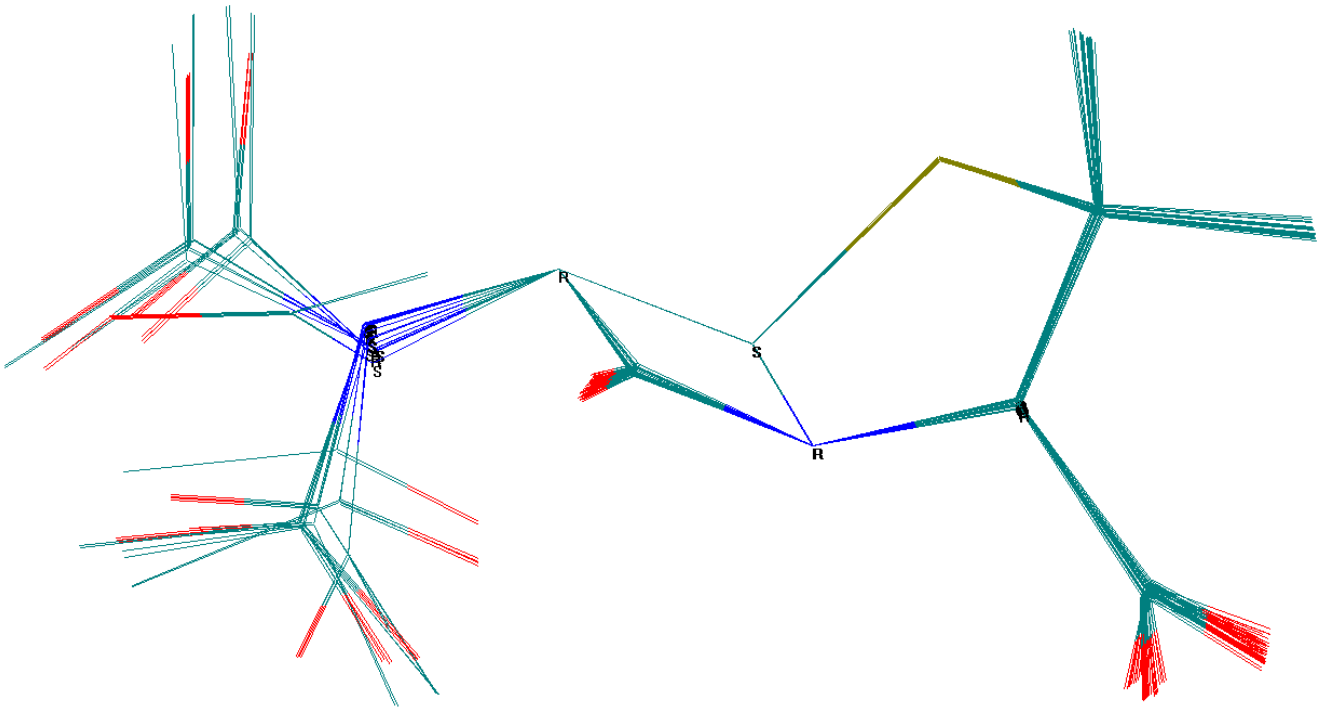


Fig. 1 b. Puckering of the thiazolidinic ring in PM3 HyperChem 7.5 (without the hydrogen atoms)

Table 3.

PM3-ID for conformers obtained by MOPAC12, standard formation enthalpy Δ_fH^0, ν_0, dihedral angles 5-1-2-3; 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14.

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
PM3-01	-144.8359	-9.832	-11.036	-3.135	-23.299	R	*syn*	27.56
PM3-02	-144.6097	-9.636	11.788	-3.044	22.414	S	*syn*	21.50
PM3-03	-144.3828	-10.576	-158.876	-2.566	22.931	S	*anti*	31.59
PM3-04	-144.3402	-9.401	-10.763	-2.984	-23.370	R	*syn*	26.13
PM3-05	-144.3083	-10.246	159.374	-3.163	-22.668	R	*anti*	26.06
PM3-06	-144.1829	-9.952	-12.847	-3.062	-23.307	R	*syn*	24.49
PM3-07	-144.1281	-9.277	12.076	-2.892	22.458	S	*syn*	23.34
PM3-08	-144.0397	-9.537	14.414	-3.150	22.400	S	*syn*	26.45
PM3-09	-143.8172	-10.434	-156.886	-2.384	23.069	S	*anti*	30.67
PM3-10	-143.6855	-10.100	159.214	-2.924	-22.606	R	*anti*	24.81
PM3-11	-143.6876	-9.535	-12.438	-2.923	-23.352	R	*syn*	26.20
PM3-12	-143.5527	-9.137	14.646	-2.997	22.464	S	*syn*	25.38
PM3-13	-142.0756	-10.610	-10.695	-1.603	-21.936	R	*syn*	33.27
PM3-14	-141.8813	-9.469	11.417	-4.074	26.363	S	*syn*	35.73
PM3-15	-141.7056	-11.408	12.943	-0.813	20.136	S	*syn*	35.23
PM3-16	-141.5014	-10.498	9.599	-1.776	22.697	S	*syn*	34.17
PM3-17	-141.4437	-10.504	-10.970	-1.302	-21.843	R	*syn*	33.49
PM3-18	-141.3620	-8.900	11..668	-3.962	26.359	S	*syn*	35.27
PM3-19	-141.0815	-11.248	12.808	-0.516	20.120	S	*syn*	34.70
PM3-20	-140.9252	-10.434	9.190	-1.588	22.833	S	*syn*	34.88
PM3-21	-140.7363	-11.408	-159.060	-1.436	23.325	S	*anti*	29.54
PM3-22	-140.5919	-11.361	158.811	-0.664	-23.067	R	*anti*	31.26
PM3-23	-140.3941	-10.523	159.690	-0.679	-23.144	R	*anti*	33.87
PM3-24	-140.3349	-10.592	164.342	-1.579	-23.399	R	*anti*	33.33
PM3-25	-140.3315	-10.788	-155.265	-0.969	22.977	S	*anti*	31.25
PM3-26	-140.1565	-10.499	164.357	-1.552	-23.305	R	*anti*	34.50
PM3-27	-139.5191	-10.249	-160.829	2.444	21.476	S	*anti*	33.25
PM3-28	-139.3334	-10.042	-161.002	-2.362	21.216	S	*anti*	34.81
PM3-29	-137.8158	-10.499	148.377	-3.362	32.696	S	*anti*	36.05
PM3-30	-137.1424	-9.949	148.678	-3.019	32.658	S	*anti*	34.37
Mean		**-10.222**		**-2.135**				**30.77**
SD		0.672		1.329				4.38

$\Delta(\Delta_fH^0) = 7.6934$kcal·mol^{-1}

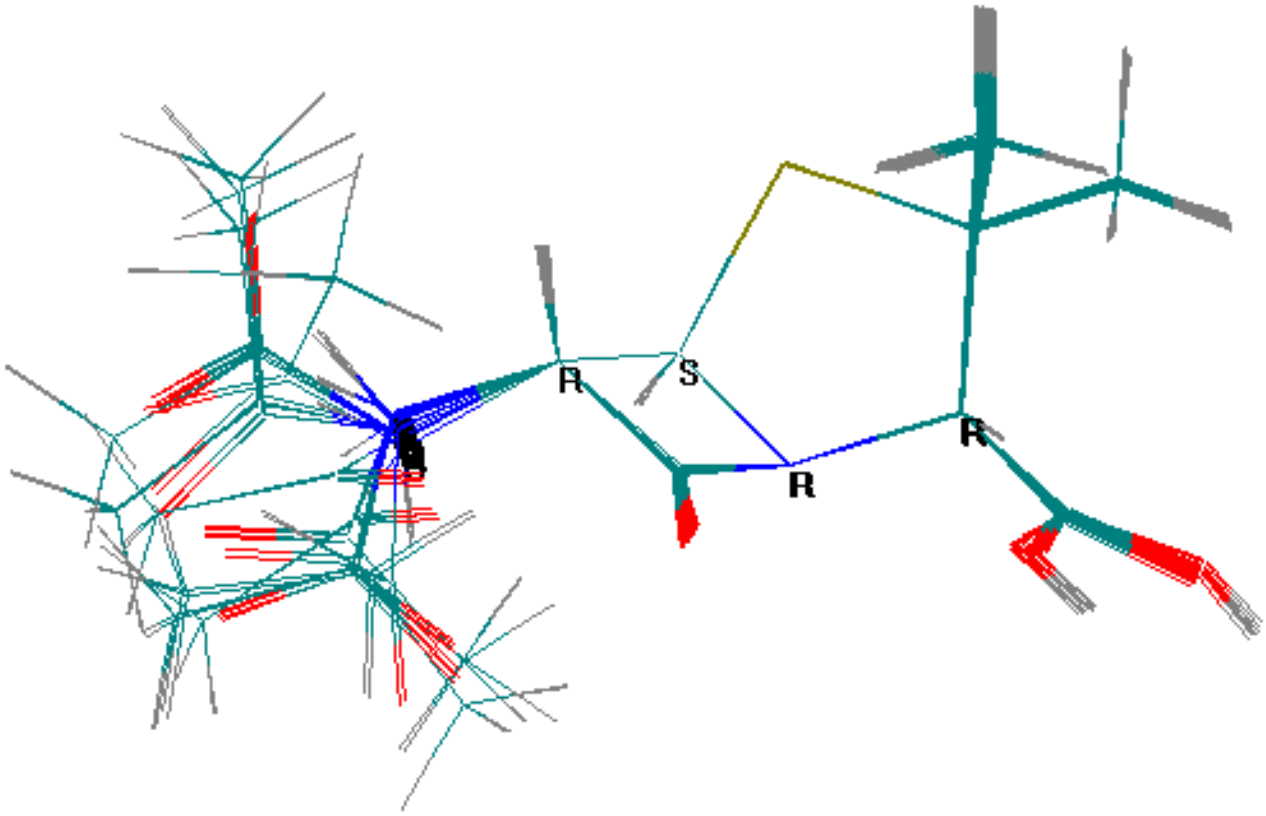


Fig. 2 a. Puckering of the thiazolidinic ring in PM3 MOPAC12 (with the hydrogen atoms)

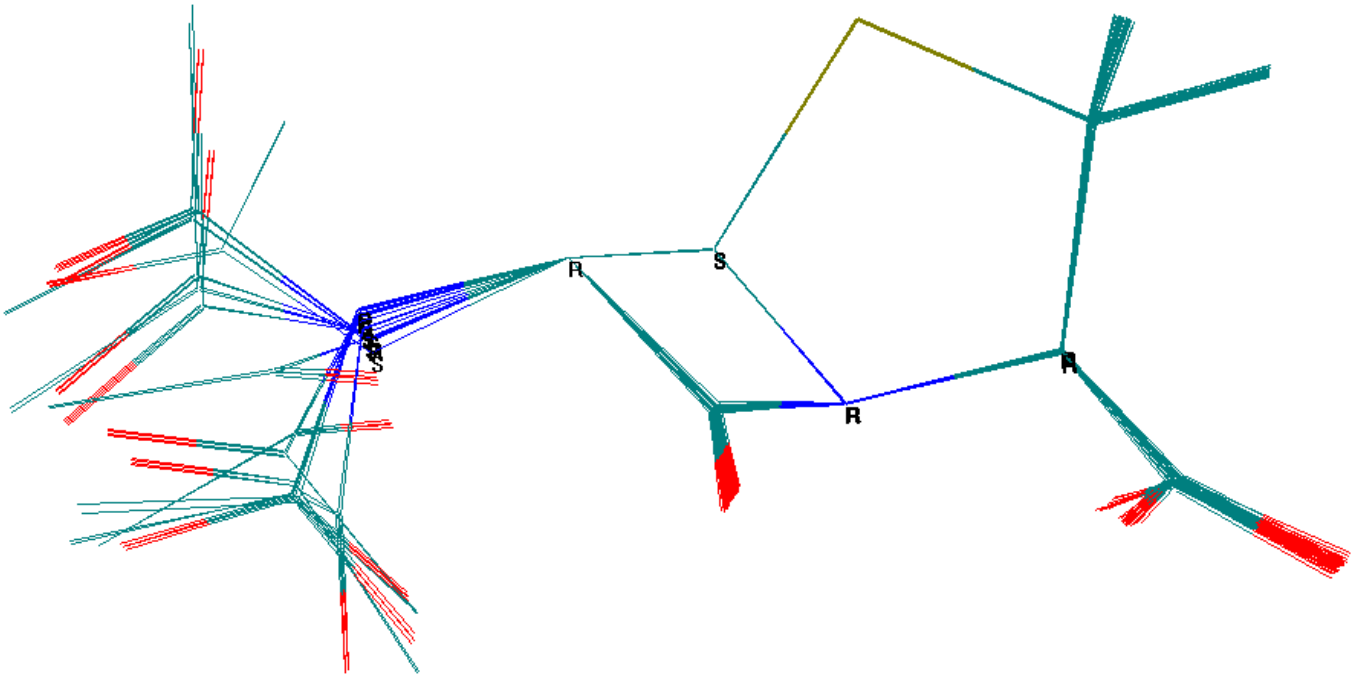


Fig. 2 b. Puckering of the thiazolidinic ring in PM3 MOPAC12 (without the hydrogen atoms)

Table 4a.

PM6 distinct conformers obtained by MOPAC12, standard formation enthalpy (Δ_fH^0), ν_0, dihedral angles 5-1-2-3, 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14.

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
PM6-03/PM6-01	-170.0039	-8.989	-178.217	-5.319	2.289	S	*anti*	30.88
PM6-09/PM6-02	-168.8314	-10.203	-177.586	-5.407	3.125	S	*anti*	31.64
PM6-01/PM6-03	-168.6504	-7.706	2.466	-5.601	1.937	S	*syn*	14.95
PM6-15/PM6-04	-168.1605	-9.219	0.669	-3.938	4.594	S	*syn*	31.34
PM6-04/PM6-05	-167.6045	-9.130	4.079	-5.766	3.405	S	*syn*	15.60
PM6-20/PM6-06	-167.0480	-10.654	0.353	-4.119	4.669	S	*syn*	33.31
PM6-29/PM6-07	-166.9291	-8.379	176.784	-3.321	-7.518	R	*anti*	22.28
PM6-25/PM6-08	-166.3517	-9.323	176.726	-3.869	-7.678	R	*anti*	25.86

Table 4b.

PM6-ID for conformers obtained by MOPAC12, standard formation enthalpy (Δ_fH^0), ν_0, dihedral angles 5-1-2-3, 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14.

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
PM6-01	-170.0039	-8.989	-178.217	-5.319	2.289	S	*anti*	30.88
PM6-02	-168.8314	-10.203	-177.586	-5.407	3.125	S	*anti*	31.64
PM6-03	-168.6504	-7.706	2.466	-5.601	1.937	S	*syn*	14.95
PM6-04	-168.1605	-9.219	0.669	-3.938	4.594	S	*syn*	31.34
PM6-05	-167.6045	-9.130	4.079	-5.766	3.405	S	*syn*	15.60
PM6-06	-167.0480	-10.654	0.353	-4.119	4.669	S	*syn*	33.31
PM6-07	-166.9291	-8.379	176.784	-3.321	-7.518	R	*anti*	22.28
PM6-08	-166.3517	-9.323	176.726	-3.869	-7.678	R	*anti*	25.86

$$\Delta(\Delta_fH^0) = 3.6541 \text{kcal·mol}^{-1}$$

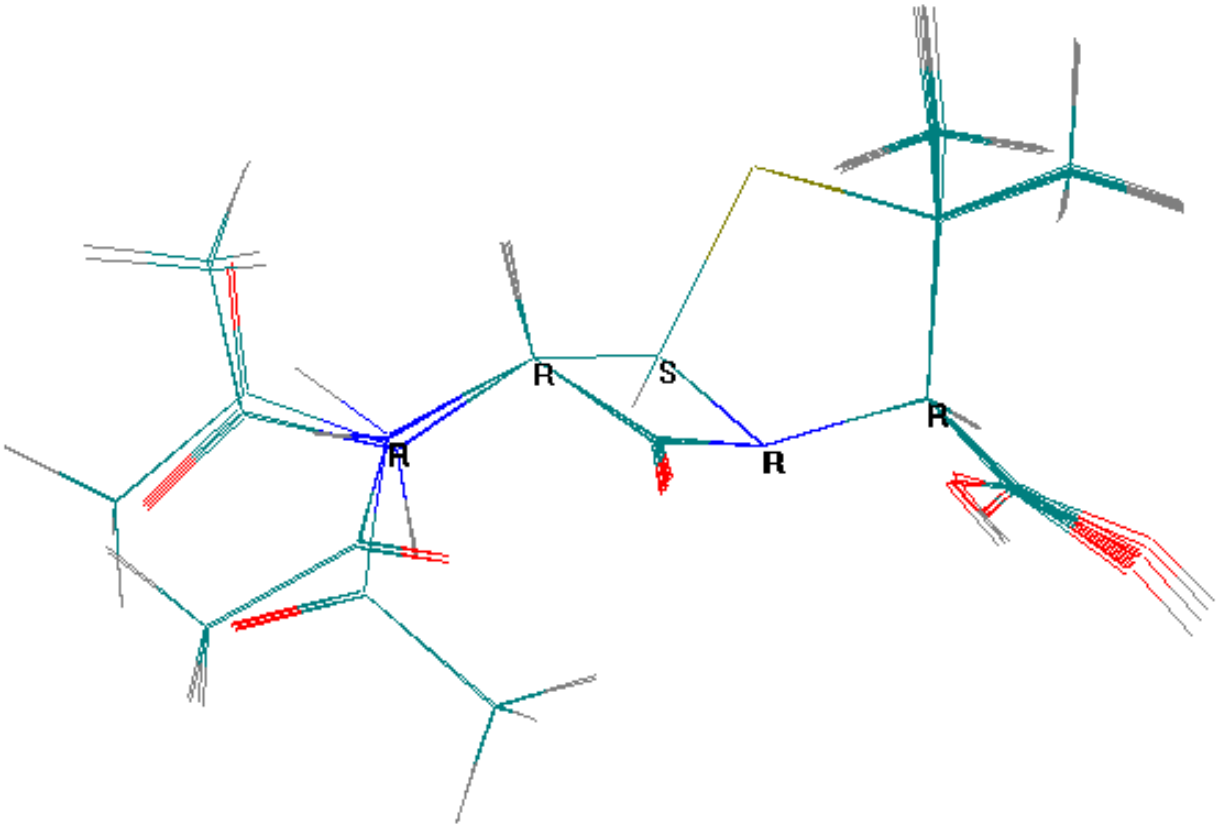


Fig. 3 a. Puckering of the thiazolidinic ring in PM6 MOPAC12 (with the hydrogen atoms)

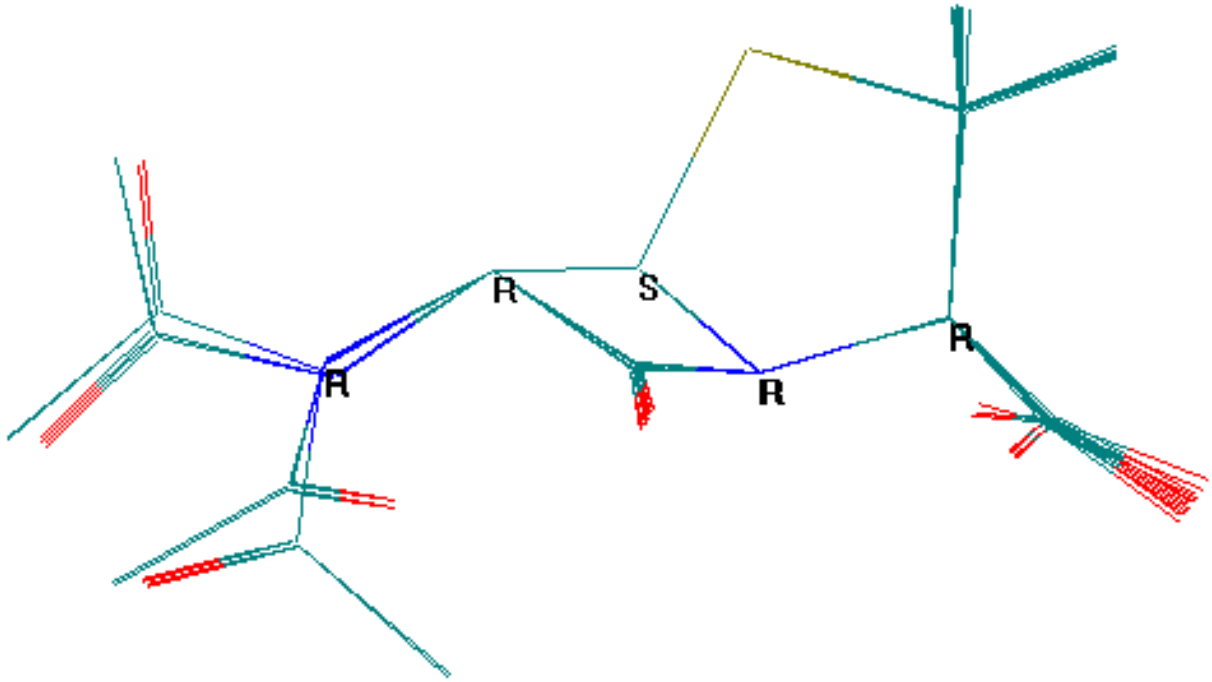


Fig. 3 b. Puckering of the thiazolidinic ring in PM6 MOPAC12 (without the hydrogen atoms)

Table 5a.

PM7 distinct conformers obtained by MOPAC12, standard formation enthalpy (Δ_fH^0), ν_0, dihedral angles 5-1-2-3, 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14.

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
PM7-03/PM7-01	-156.1798	-11.147	-177.605	-5.680	3.087	S	*anti*	30.62
PM7-09/PM7-02	-155.2229	-11.108	-177.913	-5.864	2.984	S	*anti*	30.21
PM7-01/PM7-03	-154.4311	-10.561	3.680	-5.796	3.716	S	*syn*	15.70
PM7-13/PM7-04	-153.9480	-11.180	-0.516	-4.298	3.187	S	*syn*	35.64
PM7-04/PM7-05	-153.6369	-10.326	3.784	-6.017	3.467	S	*syn*	15.64
PM7-17/PM7-06	-153.0885	-11.097	-0.304	-4.587	4.590	S	*syn*	35.94
PM7-29/PM7-07	-152.0008	-11.392	179.862	-4.386	2.993	S	*anti*	34.36
PM7-21/PM7-08	-151.8152	-11.315	176.755	-2.340	-7.323	R	*anti*	24.95
PM7-23/PM7-09	-151.3734	-9.961	175.860	-3.057	-8.400	R	*anti*	28.01

Table 5b.

PM7-ID for conformers obtained by MOPAC12, standard formation enthalpy (Δ_fH^0), ν_0, dihedral angles 5-1-2-3, 28-14-15-17, 4-5-6-7; and improper dihedral angles 6.15.28.14.

ID	Δ_fH^0 kcal·mol^{-1}	(°)				N14 Chir.	17, 28 Conf.	ν_0 cm^{-1}
		5-1-2-3	28-14-15-17	4-5-6-7	6.15.28.14			
PM7-01	-156.1798	-11.147	-177.605	-5.680	3.087	S	*anti*	30.62
PM7-02	-155.2229	-11.108	-177.913	-5.864	2.984	S	*anti*	30.21
PM7-03	-154.4311	-10.561	3.680	-5.796	3.716	S	*syn*	15.70
PM7-04	-153.9480	-11.180	-0.516	-4.298	3.187	S	*syn*	35.64
PM7-05	-153.6369	-10.326	3.784	-6.017	3.467	S	*syn*	15.64
PM7-06	-153.0885	-11.097	-0.304	-4.587	4.590	S	*syn*	35.94
PM7-07	-152.0008	-11.392	179.862	-4.386	2.993	S	*anti*	34.36
PM7-08	-151.8152	-11.315	176.755	-2.340	-7.323	R	*anti*	24.95
PM7-09	-151.3734	-9.961	175.860	-3.057	-8.400	R	*anti*	28.01

$\Delta(\Delta_fH^0) = 4.8064$kcal·mol^{-1}

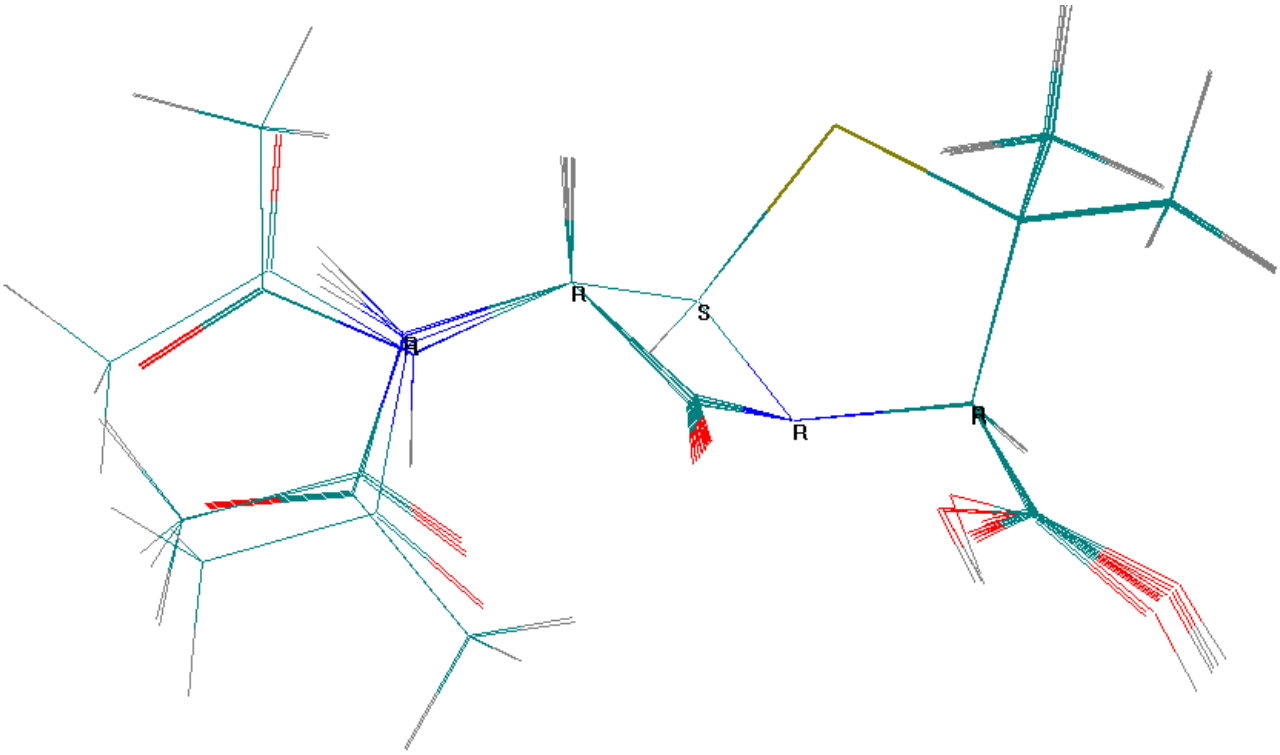


Fig. 4 a. Puckering of the thiazolidinic ring in PM7 MOPAC12 (with the hydrogen atoms)

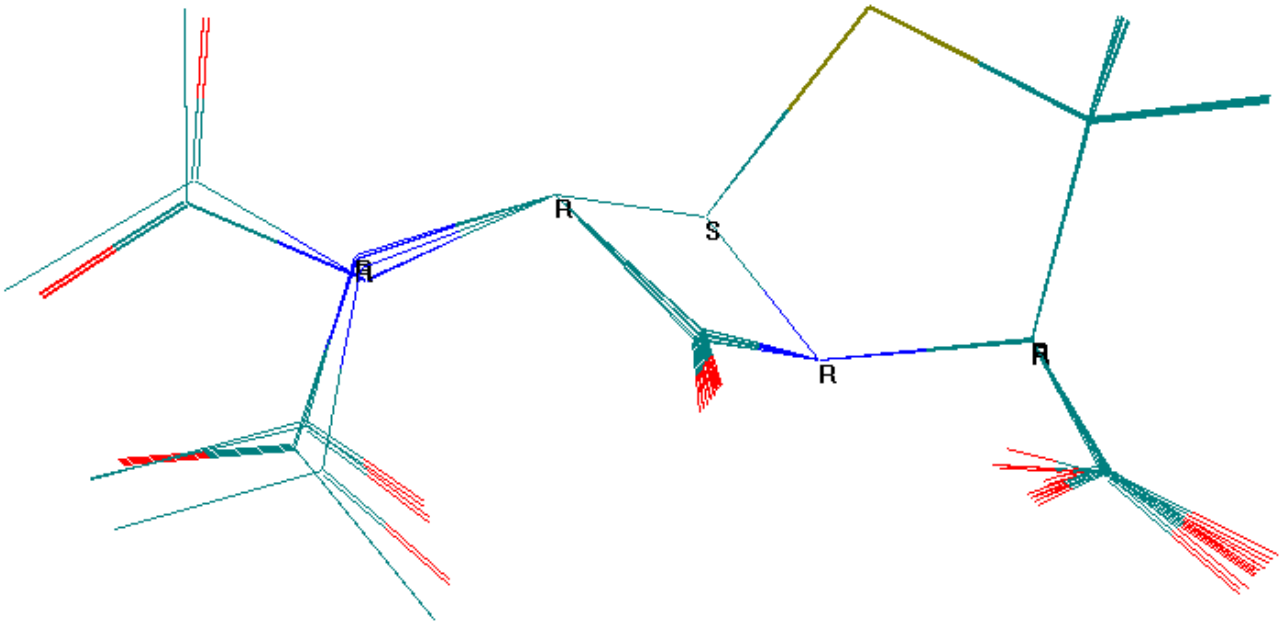


Fig. 4 b. Puckering of the thiazolidinic ring in PM7 MOPAC12 (without the hydrogen atoms)

Table 6.

Experimental geometric features (obtained from X-ray data) for several penicillins [a1-a6]

Penicillin[b]	(°) 5-1-2-3	5-4-3-2	28-14-15-17	4-5-6-7	6.15.28.14	N14 chiral.	O17, H28 Conform.
AMCILL [a1-a3,c]	*-40.28*[c]	*-9.74*[c]	*181.12*	*4.35*	*2.64*	*planar*	*anti*
BEBCAM[a1]	*15.68*	*34.36*	*183.01*	*8.22*	*0.00*	*planar*	*anti*
BENPEN10[a1]	*17.58*	*40.26*	*185.87*	*7.82*	*-1.14*	*planar*	*anti*
BPENCE10[a1]	*21.08*	*38.80*	*170.56*	*7.10*	*-13.42*	R	*anti*
BZPEN01[a1]	*16.05*	*32.45*	*199.07*	*5.32*	*13.55*	S	*anti*
CMIPEN[a1]	*14.13*	*39.14*	*182.79*	*10.14*	*0.77*	*planar*	*anti*
DCLOXL[a1]	*12.84*	*40.80*	*161.29*	*11.49*	*-10.91*	R	*anti*
FECPAE[a1]	*16.90*	*36.57*	*169.88*	*7.49*	*-8.30*	R	*anti*
JOTLAF[a1]	*22.21*	*37.52*	*174.59*	*6.38*	*-6.58*	R	*anti*
MECILIN[a1,d]	*-36.85*	*0.16*	-	*13.53*	-	-	-
METHIC[a1,c]	*-40.91*[c]	*-2.87*[c]	*178.71*	*13.98*	*1.15*	*planar*	*anti*
PMEPEN[a1,c]	*-23.54*[c]	*-35.58*[c]	*172.54*	*-5.54*	*0.00*	*planar*	*anti*
PMEPEN01[a4]	*22.12*	*36.42*	*172.25*	*5.01*	*-8.98*	R	*anti*
PRPENG[a5]	*-31.51*	*-8.85*	*175.76*	*-13.22*	*-8.83*	R	*anti*
VUKHUE[a6,e]	*9.53*	*34.16*	*179.69*	*10.45*	*6.46*[d]	-	-
VUKJAM[a6,e]	*22.05*	*37.59*	*3.71*	*2.44*	*3.18*[d]	-	-

[a1] experimental geometries and notation code are those taken from the **Cambridge Crystallographic Data Centre 2006-2010,** http://www.ccdc.cam.ac.uk/services/structure_deposit; [a2] I. Csoregh, T-B. Palm, Acta Crystallogr. Sect. B: Struct. Crystallogr. Cryst Chem **33** (1977) 2169-2171; [a3] M. O. Boles, R. J. Girven, Acta Cryst. **B32** (1976) 2279-2284; [a4] W. Shin, S. W. Cho, Acta Cryst. **C48** (1992) 1447-1449; [a5] D. D. Dexter, J. M. van der Veen, J. Chem. Soc. Perkin Trans. **1** (1978) 185 – 190; [a6] Z. Urbanczyk-Lipkowska, P. Eda, Acta Cryst. **C48** (1992) 2167-2172

[b] chemical structure, IUPAC name and trade name of the penicillins following in Tab. 1, are given in the supplementary material 01.

[c] thiazolidine ring has a different puckering in comparison to other rings (both 5-1-2-3 and 5-4-3-2 dihedral angles are negative)

[d] do not have pseudochirality at the N14 atom because of the N14=C15 double bond

[e] do not have pseudochirality at the N14 atom because two substitutes are identical

Table 7a.

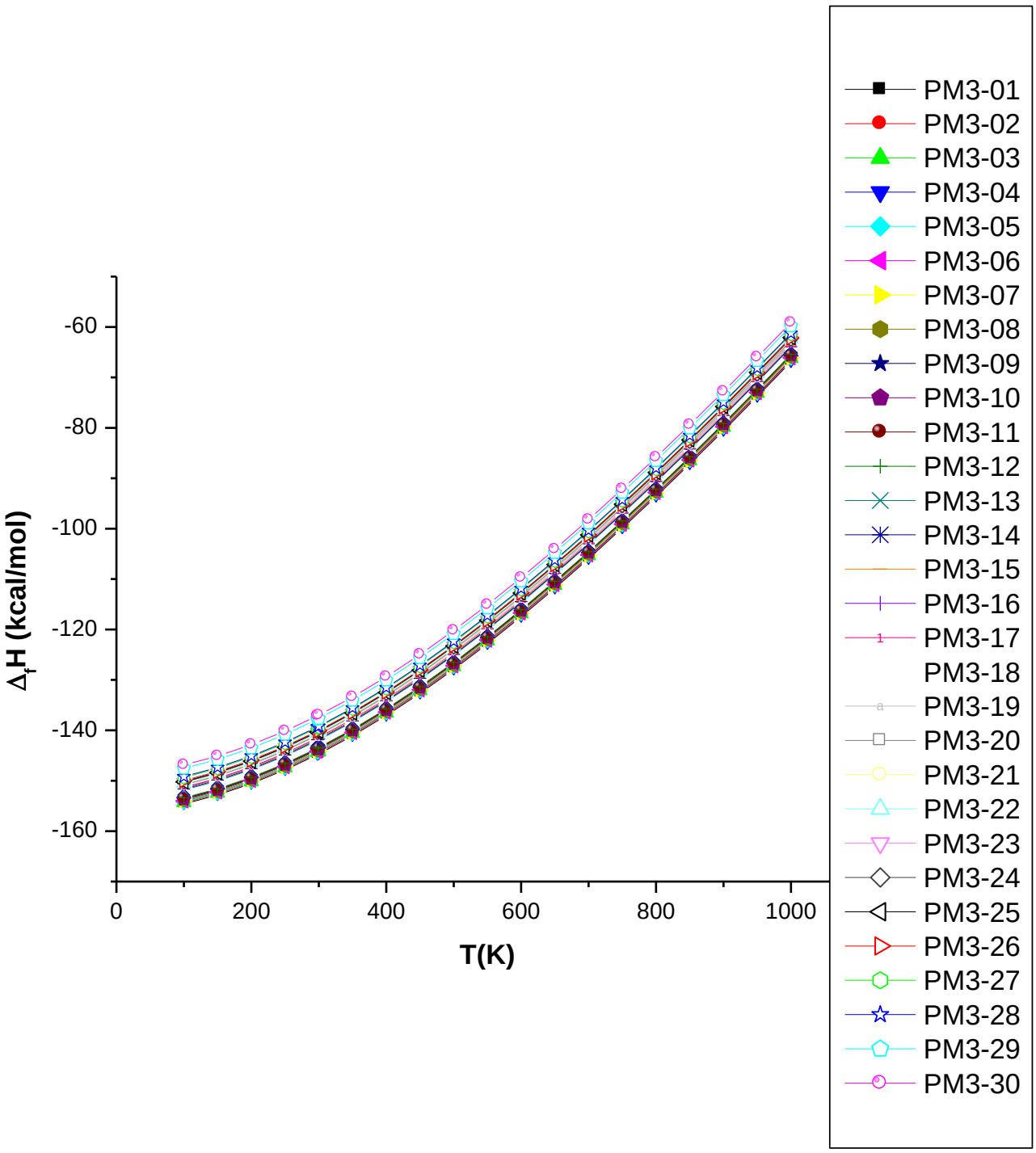
$\Delta_f H$(kcal·mol^{-1}) = f(T) computed by PM3-M12

Conf / T(K)	PM3-01	PM3-02	PM3-03	PM3-04	PM3-05	PM3-06	PM3-07	PM3-08	PM3-09	PM3-10	PM3-11	PM3-12	PM3-13	PM3-14	PM3-15
100	-154.631	-154.430	-154.300	-154.133	-154.216	-154.032	-153.946	-153.899	-153.731	-153.592	-153.532	-153.411	-151.829	-151.661	-151.492
150	-152.836	-152.627	-152.470	-152.340	-152.389	-152.226	-152.145	-152.091	-151.904	-151.768	-151.729	-151.605	-150.059	-149.875	-149.719
200	-150.574	-150.359	-150.177	-150.079	-150.098	-149.950	-149.878	-149.812	-149.612	-149.478	-149.455	-149.327	-147.811	-147.617	-147.462
250	-147.861	-147.640	-147.435	-147.366	-147.359	-147.223	-147.159	-147.082	-146.870	-146.737	-146.728	-146.596	-145.103	-144.906	-144.743
298	-144.836	-144.610	-144.383	-144.340	-144.308	-144.183	-144.128	-144.040	-143.817	-143.685	-143.688	-143.553	-142.076	-141.881	-141.706
300	-144.701	-144.475	-144.247	-144.205	-144.172	-144.047	-143.993	-143.904	-143.681	-143.549	-143.552	-143.417	-141.940	-141.746	-141.570
350	-141.101	-140.870	-140.620	-140.605	-140.547	-140.431	-140.388	-140.286	-140.054	-139.923	-139.935	-139.798	-138.334	-138.145	-137.954
400	-137.083	-136.848	-136.575	-136.585	-136.503	-136.396	-136.365	-136.249	-136.009	-135.878	-135.899	-135.760	-134.307	-134.124	-133.917
450	-132.676	-132.439	-132.144	-132.178	-132.073	-131.972	-131.955	-131.825	-131.576	-131.446	-131.475	-131.335	-129.889	-129.713	-129.491
500	-127.915	-127.675	-127.359	-127.417	-127.289	-127.195	-127.192	-127.047	-126.792	-126.661	-126.697	-126.556	-125.117	-124.947	-124.711
550	-122.835	-122.593	-122.256	-122.336	-122.187	-122.098	-122.109	-121.950	-121.689	-121.558	-121.601	-121.459	-120.026	-119.861	-119.612
600	-117.466	-117.223	-116.867	-116.967	-116.798	-116.715	-116.739	-116.567	-116.300	-116.169	-116.217	-116.075	-114.647	-114.487	-114.226
650	-111.838	-111.594	-111.221	-111.339	-111.152	-111.073	-111.109	-110.925	-110.653	-110.523	-110.576	-110.433	-109.009	-108.853	-108.582
700	-105.976	-105.730	-105.341	-105.476	-105.273	-105.198	-105.246	-105.050	-104.773	-104.643	-104.700	-104.557	-103.137	-102.985	-102.704
750	-99.901	-99.654	-99.250	-99.401	-99.183	-99.112	-99.170	-98.963	-98.682	-98.552	-98.613	-98.470	-97.053	-96.905	-96.615
800	-93.633	-93.385	-92.967	-93.132	-92.900	-92.832	-92.900	-92.684	-92.399	-92.269	-98.613	-92.190	-90.775	-90.630	-90.333
850	-87.187	-86.938	-86.509	-86.686	-86.441	-86.377	-86.454	-86.228	-85.940	-85.810	-85.87	-85.735	-84.322	-84.179	-83.874
900	-80.579	-80.330	-79.889	-80.078	-79.822	-79.760	-79.845	-79.611	-79.320	-79.190	-79.261	-79.118	-77.706	-77.566	-77.255
950	-73.822	-73.573	-73.121	-73.321	-73.055	-72.994	-73.088	-72.846	-72.553	-72.423	-72.496	-72.352	-70.942	-70.804	-70.487
1000	-66.928	-66.678	-66.217	-66.427	-66.151	-66.093	-66.193	-65.945	-65.648	-65.518	-65.594	-65.450	-64.041	-63.905	-63.582

Table 7b.

$\Delta_f\mathbf{H}$(kcal·mol^{-1}) = f(T) computed by PM3-M12

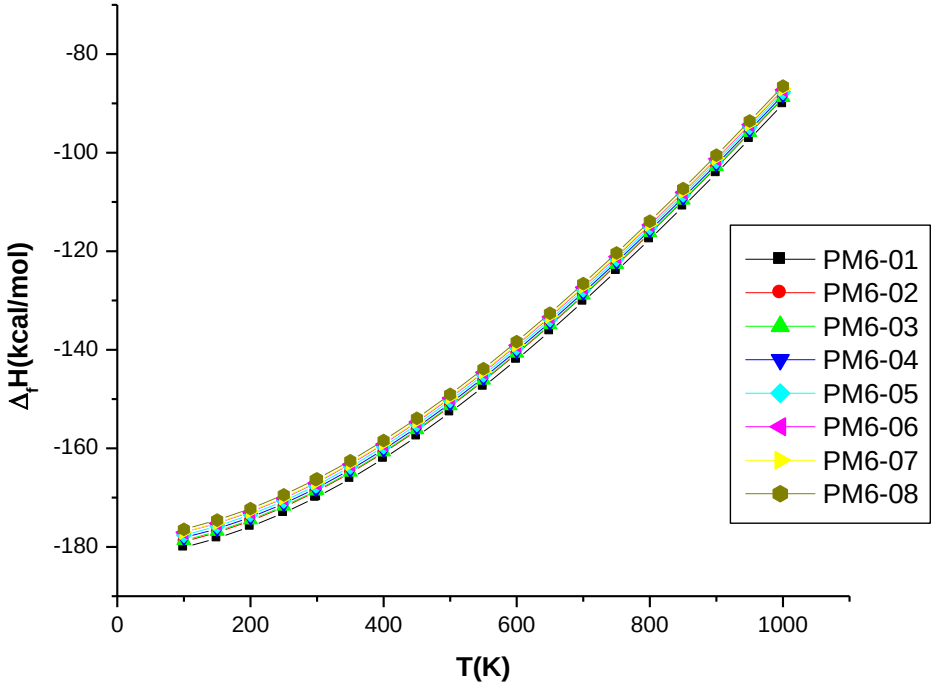
Conf / T(K)	PM3-16	PM3-17	PM3-18	PM3-19	PM3-20	PM3-21	PM3-22	PM3-23	PM3-24	PM3-25	PM3-26	PM3-27	PM3-28	PM3-29	PM3-30
100	-151.367	-151.196	-151.141	-150.866	-150.785	-150.655	-150.518	-150.309	-150.153	-150.252	-149.970	-149.385	-149.194	-147.564	-146.889
150	-149.559	-149.428	-149.357	-149.095	-148.981	-148.826	-148.688	-148.484	-148.352	-148.425	-148.172	-147.573	-147.386	-145.787	-145.114
200	-147.281	-147.181	-147.100	-146.839	-146.704	-146.533	-146.393	-146.193	-146.084	-146.133	-145.906	-145.292	-145.107	-143.537	-142.866
250	-144.549	-144.472	-144.388	-144.120	-143.973	-143.791	-143.649	-143.450	-143.366	-143.389	-143.188	-142.561	-142.376	-140.835	-140.163
298	-141.501	-141.444	-141.362	-141.081	-140.925	-140.736	-140.592	-140.394	-140.335	-140.331	-140.156	-139.519	-139.333	-137.816	-137.142
300	-141.365	-141.308	-141.227	-140.946	-140.789	-140.600	-140.456	-140.258	-140.200	-140.195	-140.021	-139.383	-139.198	-137.681	-137.008
350	-137.739	-137.701	-137.624	-137.329	-137.163	-136.969	-136.822	-136.626	-136.594	-136.561	-136.415	-135.768	-135.582	-134.083	-133.408
400	-133.693	-133.672	-133.602	-133.291	-133.116	-132.918	-132.771	-132.575	-132.569	-132.509	-132.389	-131.735	-131.548	-130.063	-129.387
450	-129.258	-129.254	-129.190	-128.864	-128.681	-128.480	-128.331	-128.136	-128.155	-128.069	-127.975	-127.314	-127.128	-125.651	-124.974
500	-124.469	-124.481	-124.423	-124.083	-123.892	-123.690	-123.539	-123.345	-123.386	-123.277	-123.207	-122.540	-122.354	-120.883	-120.205
550	-119.361	-119.389	-119.336	-118.984	-118.785	-118.581	-118.430	-118.237	-118.298	-118.166	-118.119	-117.447	-117.261	-115.795	-115.116
600	-113.967	-114.009	-113.961	-113.598	-113.391	-113.186	-113.034	-112.842	-112.922	-112.771	-112.743	-112.067	-111.881	-110.418	-109.738
650	-108.316	-108.370	-108.327	-107.953	-107.739	-107.534	-107.381	-107.190	-107.286	-107.117	-107.107	-106.428	-106.242	-104.781	-104.101
700	-102.431	-102.498	-102.458	-102.075	-101.855	-101.650	-101.495	-101.305	-101.415	101.232	-101.237	-100.555	-100.369	-98.910	-98.229
750	-96.336	-96.413	-96.377	-95.985	-95.760	-95.554	-95.399	-95.210	-95.332	-95.136	-95.154	-94.469	-94.284	-92.827	-92.145
800	-90.048	-90.136	-90.102	-89.703	-89.472	-89.267	-89.111	-88.923	-89.056	-88.848	-88.878	-88.191	-88.006	-86.550	-85.868
850	-83.585	-83.681	-83.650	-83.244	-83.009	-82.805	-82.648	-82.460	-82.602	-82.385	-82.425	-81.735	-81.550	-80.097	-79.414
900	-76.961	-77.066	-77.037	-76.624	-76.385	-76.181	-76.024	-75.837	-75.987	-75.761	-75.809	-75.118	-74.933	-73.481	-72.798
950	-70.189	-70.301	-70.274	-69.856	-69.613	-69.411	-69.252	-69.065	-69.222	-68.989	-69.045	-68.352	-68.168	-66.717	-66.034
1000	-63.281	-63.400	-63.375	-62.951	-62.705	-62.504	-62.345	-62.158	-62.321	-62.082	-62.144	-61.450	-61.265	-59.817	-59.132



Functional dependencies $\Delta_f H$ graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM3-M12

Table 8.
ΔH$_f$(kcal•mol^{-1}) = f(T) computed by PM6-M12

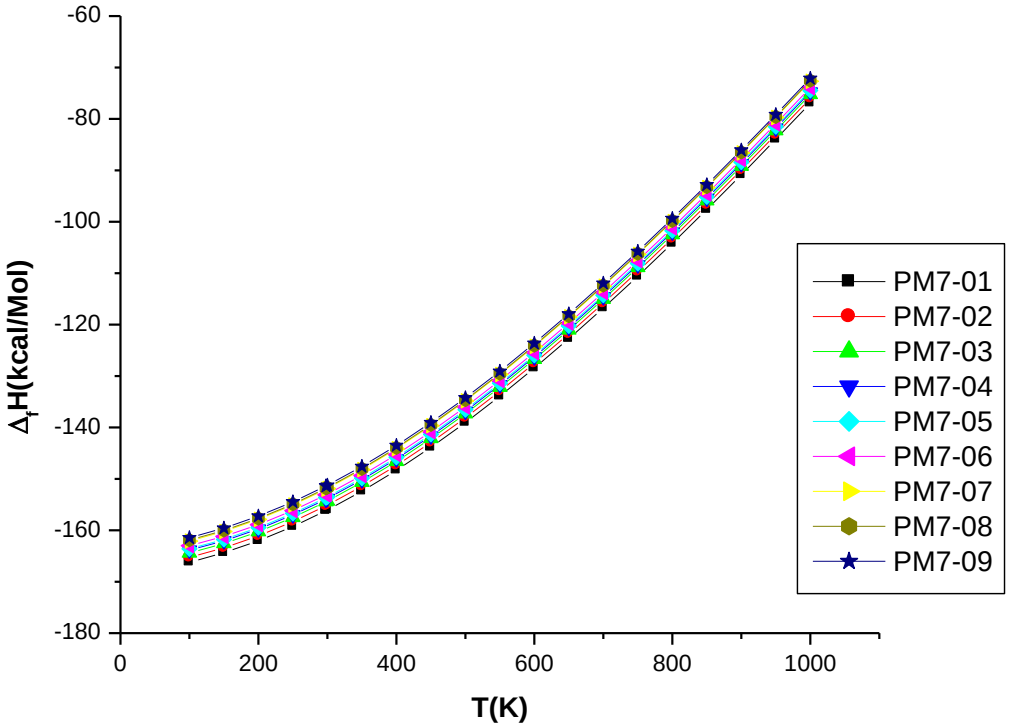
Conf / T(K)	PM6-01	PM6-02	PM6-03	PM6-04	PM6-05	PM6-06	PM6-07	PM6-08
100	-180.125	-178.953	-178.710	-178.145	-177.668	-177.029	-177.013	-176.442
150	-178.244	-177.072	-176.849	-176.316	-175.806	-175.202	-175.145	-174.573
200	-175.897	-174.726	-174.521	-174.009	-173.478	-172.896	-172.809	-172.236
250	-173.105	-171.933	-171.743	-171.244	-170.698	-170.132	-170.025	-169.450
298	-170.004	-168.831	-168.650	-168.160	-167.605	-167.048	-166.929	-166.352
300	-169.866	-168.693	-168.513	-168.023	-167.467	-166.910	-166.791	-166.214
350	-166.182	-165.010	-164.836	-164.352	-163.789	-163.240	-163.112	-162.533
400	-162.073	-160.901	-160.732	-160.251	-159.685	-159.140	-159.006	-158.426
450	-157.567	-156.396	-156.231	-155.751	-155.184	-154.642	-154.502	-153.921
500	-152.698	-151.528	-151.366	-150.886	-150.319	-149.778	-149.635	-149.054
550	-147.498	-146.329	-146.170	-145.691	-145.124	-144.584	-144.437	-143.856
600	-142.001	-140.833	-140.675	-140.196	-139.629	-139.090	-138.941	-138.360
650	-136.233	-135.066	-134.910	-134.430	-133.865	-133.326	-133.174	-132.593
700	-130.221	-129.055	-128.900	-128.419	-127.856	-127.317	-127.163	-126.582
750	-123.986	-122.822	-122.669	-122.187	-121.625	-121.085	-120.930	-120.348
800	-117.551	-116.387	-116.235	-115.752	-115.192	-114.652	-114.494	-113.913
850	-110.932	-109.769	-109.618	-109.134	-108.575	-108.034	-107.876	-107.294
900	-104.145	-102.983	-102.833	-102.348	-101.791	-101.249	-101.089	-100.508
950	-97.206	-96.044	-95.896	-95.409	-94.854	-94.312	-94.150	-93.569
1000	-90.127	-88.966	-88.818	-88.330	-87.777	-87.234	-87.071	-86.490



Functional dependencies **Δ$_f$H** graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM6-M12

Table 9.
$\Delta_f H$(kcal•mol^{-1}) = f(T) computed by PM7-M12

Conf / T(K)	PM7-01	PM7-02	PM7-03	PM7-04	PM7-05	PM7-06	PM7-07	PM7-08	PM7-09
100	-166.221	-165.262	-164.401	-163.851	-163.604	-162.981	-162.097	-161.894	-161.437
150	-164.360	-163.403	-162.565	-162.044	-161.769	-161.178	-160.222	-160.024	-159.574
200	-162.031	-161.074	-160.256	-159.754	-159.462	-158.891	-157.878	-157.684	-157.239
250	-159.257	-158.300	-157.498	-157.008	-156.703	-156.147	-155.090	-154.901	-154.458
298	-156.180	-155.223	-154.431	-153.948	-153.637	-153.088	-152.001	-151.815	-151.373
300	-156.043	-155.086	-154.294	-153.812	-153.500	-152.952	-151.863	-151.678	-151.236
350	-152.394	-151.437	-150.654	-150.175	-149.860	-149.317	-148.202	-148.021	-147.581
400	-148.327	-147.371	-146.593	-146.116	-145.800	-145.261	-144.125	-143.948	-143.509
450	-143.869	-142.915	-142.141	-141.665	-141.349	-140.811	-139.657	-139.484	-139.048
500	-139.051	-138.098	-137.328	-136.851	-136.537	-136.000	-134.830	-134.662	-134.228
550	-133.904	-132.953	-132.185	-131.708	-131.396	-130.859	-129.675	-129.512	-129.080
600	-128.459	-127.510	-126.744	-126.266	-125.956	-125.419	-124.223	-124.064	-123.634
650	-122.743	-121.795	-121.031	-120.553	-120.245	-119.708	-118.501	-118.346	-117.918
700	-116.781	-115.835	-115.072	-114.593	-114.287	-113.750	-112.533	-112.382	-111.956
750	-110.595	-109.650	-108.889	-108.409	-108.105	-107.567	-106.343	-106.195	-105.770
800	-104.205	-103.262	-102.502	-102.020	-101.719	-101.180	-99.949	-99.805	-99.381
850	-97.630	-96.687	-95.929	-95.446	-95.147	-94.607	-93.370	-93.229	-92.806
900	-90.885	-89.943	-89.186	-88.701	-88.405	-87.864	-86.622	-86.483	-86.062
950	-83.985	-83.044	-82.287	-81.802	-81.508	-80.966	-79.719	-79.583	-79.163
1000	-76.943	-76.003	-75.247	-74.760	-74.468	-73.926	-72.675	-72.541	-72.121



Functional dependencies **$\Delta_f H$** graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM7-M12