

Supplementary material for:

**ENTROPIC EFFECT AND THERMODYNAMIC PROPERTIES FOR THE
CONFORMERS OF (3R,5S,6R)-6-ACETYLAMIDOPENICILLANIC ACID
CALCULATED WITH THE PM3, PM6 AND PM7 SEMIEMPIRICAL MO
METHODS**

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Table 1a.
 $\Delta H(\text{kcal}\cdot\text{mol}^{-1}) = f(T)$ computed by PM3-M12

Conf	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
T(K)															
100	1.9894	2.0154	2.0354	1.9843	2.0442	1.9867	2.0041	1.9817	2.0283	2.038	1.9748	1.9748	1.9068	1.9197	1.891
150	3.784	3.8187	3.8653	3.777	3.8711	3.7927	3.805	3.7901	3.8553	3.8623	3.7779	3.7813	3.6764	3.7056	3.6646
200	6.0459	6.0872	6.1589	6.038	6.1619	6.0682	6.0726	6.0686	6.1476	6.1525	6.052	6.0591	5.9248	5.9637	5.9218
250	8.7586	8.8057	8.9008	8.7507	8.9015	8.7954	8.7911	8.7986	8.8894	8.8928	8.779	8.7895	8.6328	8.6743	8.6403
298	11.7841	11.8361	11.953	11.7769	11.952	11.8357	11.822	11.8414	11.942	11.9447	11.8197	11.8331	11.6602	11.6994	11.6778
300	11.9191	11.9712	12.0891	11.9119	12.088	11.9713	11.9572	11.9771	12.0781	12.0807	11.9553	11.9688	11.7953	11.8344	11.8134
350	15.5189	15.5754	15.7159	15.5125	15.7134	15.5875	15.5621	15.5952	15.7055	15.7076	15.5721	15.588	15.4016	15.4356	15.4297
400	19.5374	19.5974	19.7604	19.5317	19.7569	19.6228	19.5847	19.6319	19.7506	19.7524	19.6079	19.6257	19.4291	19.4569	19.4667
450	23.9442	24.0071	24.1923	23.9392	24.1878	24.0466	23.995	24.0565	24.1828	24.1844	24.0321	24.0512	23.8464	23.8678	23.8926
500	28.705	28.7704	28.9768	28.7005	28.9715	28.8239	28.7586	28.8344	28.9675	28.969	28.8097	28.8298	28.6182	28.6335	28.6724
550	33.7855	33.8529	34.0794	33.7814	34.0736	33.9202	33.8414	33.931	34.0704	34.0718	33.9063	33.927	33.7098	33.7195	33.7712
600	39.1538	39.223	39.4684	39.1501	39.462	39.3035	39.2116	39.3145	39.4595	39.4608	39.2898	39.3109	39.0889	39.0936	39.1571
650	44.7816	44.8522	45.1151	44.7782	45.1082	44.9452	44.841	44.9562	45.1064	45.1076	44.9316	44.9531	44.727	44.7273	44.8014
700	50.6438	50.7156	50.9947	50.6407	50.9874	50.8203	50.7045	50.8313	50.9861	50.9872	50.8069	50.8286	50.599	50.5955	50.6791
750	56.7187	56.7916	57.0855	56.7159	57.0778	56.9071	56.7806	56.918	57.077	57.078	56.8938	56.9157	56.6831	56.6762	56.7685
800	62.9873	63.061	63.3685	62.9848	63.3605	63.1865	63.0501	63.1974	63.3601	63.3611	63.1734	63.1954	62.9604	62.9505	63.0506
850	69.4329	69.5073	69.8272	69.4307	69.8189	69.6421	69.4965	69.6528	69.8189	69.8198	69.629	69.6511	69.4141	69.4016	69.5089
900	76.0406	76.1157	76.4469	76.0387	76.4383	76.259	76.1051	76.2696	76.4388	76.4397	76.2461	76.2682	76.0295	76.0148	76.1286
950	82.7975	82.8731	83.2146	82.7959	83.2058	83.0242	82.8626	83.0347	83.2067	83.2075	83.0114	83.0336	82.7935	82.7768	82.8966
1000	89.6917	89.7677	90.1186	89.6904	90.1097	89.926	89.7574	89.9365	90.1109	90.1117	89.9134	89.9355	89.6944	89.676	89.8012

Table 1b.
 $\Delta H(\text{kcal}\cdot\text{mol}^{-1}) = f(T)$ 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	1.964	1.8964	1.9118	1.8853	1.9554	2.0352	2.0382	2.0129	1.976	2.0224	1.9612	2.0009	1.9859	1.8924	1.8849
150	3.7718	3.6636	3.6955	3.6567	3.7601	3.8645	3.8686	3.8381	3.7772	3.8492	3.7591	3.8129	3.7944	3.6695	3.6593
200	6.0498	5.9113	5.953	5.913	6.0364	6.1569	6.163	6.1296	6.0453	6.1418	6.0256	6.0939	6.0737	5.9188	5.9078
250	8.7819	8.6199	8.6642	8.6317	8.7678	8.8991	8.9075	8.8725	8.7636	8.8858	8.7436	8.8251	8.8046	8.6212	8.6107
298	11.8297	11.6484	11.6906	11.67	11.8155	11.9539	11.9643	11.9283	11.7946	11.943	11.7749	11.8671	11.8469	11.6404	11.6311
300	11.9656	11.7836	11.8256	11.8056	11.9515	12.0901	12.1005	12.0645	11.9298	12.0793	11.9101	12.0027	11.9825	11.7752	11.7659
350	15.5917	15.3912	15.4282	15.423	15.5778	15.7215	15.7337	15.6968	15.5358	15.7132	15.5164	15.6184	15.5986	15.373	15.3651
400	19.6381	19.42	19.4508	19.4608	19.6243	19.7717	19.7854	19.7477	19.5609	19.7657	19.5419	19.6515	19.6321	19.3933	19.3868
450	24.0735	23.8383	23.8628	23.8876	24.0597	24.2098	24.2248	24.186	23.9748	24.2056	23.9559	24.072	24.0527	23.805	23.7996
500	28.8623	28.611	28.6295	28.668	28.8485	29.0006	29.0167	28.9769	28.7431	28.998	28.7242	28.8458	28.8265	28.5727	28.5682
550	33.9698	33.7033	33.7163	33.7674	33.9559	34.1093	34.1266	34.0857	33.8315	34.1081	33.8123	33.9387	33.9192	33.6612	33.6576
600	39.3637	39.083	39.0912	39.1538	39.3497	39.504	39.5223	39.4804	39.2078	39.504	39.1885	39.319	39.2992	39.0382	39.0354
650	45.0153	44.7217	44.7255	44.7985	45.0013	45.1561	45.1753	45.1325	44.8437	45.1571	44.8241	44.9581	44.9381	44.6748	44.6726
700	50.8998	50.5942	50.5943	50.6766	50.8857	51.0407	51.0606	51.017	50.7141	51.0425	50.6942	50.8313	50.8111	50.5458	50.5442
750	56.9953	56.6788	56.6756	56.7664	56.9812	57.136	57.1569	57.1124	56.7971	57.1387	56.777	56.9167	56.8963	56.6293	56.6283
800	63.2829	62.9565	62.9504	63.0489	63.2687	63.4231	63.4449	63.3997	63.0738	63.4266	63.0534	63.1954	63.1748	62.9061	62.9056
850	69.7461	69.4106	69.4021	69.5075	69.7319	69.8856	69.9082	69.8624	69.5273	69.8898	69.5067	69.6507	69.6299	69.3595	69.3596
900	76.3701	76.0265	76.0157	76.1276	76.3559	76.5088	76.5321	76.4858	76.1428	76.5137	76.122	76.2679	76.2468	75.9748	75.9753
950	83.1419	82.7909	82.7783	82.8959	83.1278	83.2797	83.3038	83.257	82.9073	83.2853	82.8863	83.0337	83.0125	82.7387	82.7398
1000	90.05	89.6922	89.6779	89.8009	90.0359	90.1866	90.2115	90.1643	89.8088	90.1929	89.7878	89.9365	89.9152	89.6396	89.6412

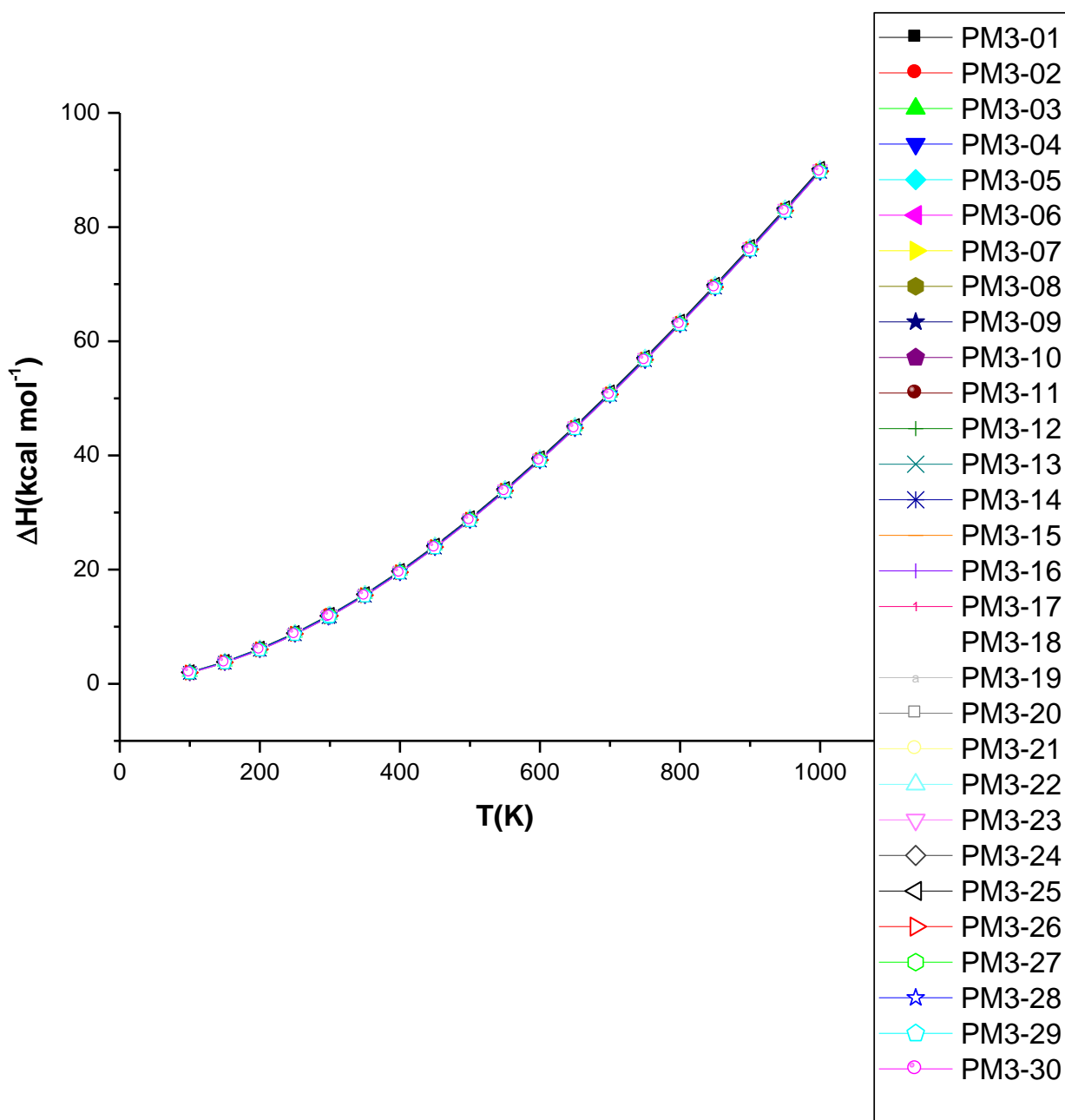


Fig. 1. Functional dependencies $\Delta H(\text{kcal}\cdot\text{mol}^{-1})$ graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM3-M12

Table 2.

M12 Polynomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of $\Delta H(\text{kcal}\cdot\text{mol}^{-1})(T)$ for distinct conformers energetic and geometric optimization with by PM3-M12, of (3R,5S,6R)-6-acetylamidopenicillanic acid

Conformer	a_0	a_1	$a_2 \cdot 10^4$	$a_3 \cdot 10^8$	r^2	SD	$F \cdot 10^{-6}$
PM3-01	0.0975	0.0078	1.1585	-3.4110	1.0000	0.0337	4.4522
PM3-02	0.1057	0.0080	1.1563	-3.4021	1.0000	0.0335	4.4896
PM3-03	0.0750	0.0085	1.1558	-3.4116	1.0000	0.0343	4.3273
PM3-04	0.0927	0.0078	1.1591	-3.4143	1.0000	0.0337	4.4307
PM3-05	0.0907	0.0084	1.1568	-3.4158	1.0000	0.0344	4.2911
PM3-06	0.0694	0.0080	1.1613	-3.4334	1.0000	0.0346	4.2392
PM3-07	0.0946	0.0080	1.1568	-3.4053	1.0000	0.0336	4.4692
PM3-08	0.0547	0.0081	1.1600	-3.4279	1.0000	0.0344	4.2823
PM3-09	0.0688	0.0085	1.1565	-3.4152	1.0000	0.0343	4.3128
PM3-10	0.0832	0.0084	1.1574	-3.4199	1.0000	0.0345	4.2746
PM3-11	0.0587	0.0080	1.1620	-3.4375	1.0000	0.0347	4.2143
PM3-12	0.0475	0.0081	1.1606	-3.4316	1.0000	0.0345	4.2582
PM3-13	0.0499	0.0072	1.1716	-3.4805	1.0000	0.0360	3.9141
PM3-14	0.0454	0.0076	1.1639	-3.4368	1.0000	0.0342	4.3232
PM3-15	0.0101	0.0074	1.1715	-3.4851	1.0000	0.0362	3.8632
PM3-16	0.0453	0.0080	1.1663	-3.4633	1.0000	0.0359	3.9420
PM3-17	0.0387	0.0072	1.1723	-3.4845	1.0000	0.0362	3.8718
PM3-18	0.0367	0.0075	1.1646	-3.4409	1.0000	0.0343	4.2986
PM3-19	0.0045	0.0074	1.1722	-3.4889	1.0000	0.0365	3.8181
PM3-20	0.0389	0.0079	1.1670	-3.4671	1.0000	0.0360	3.9187
PM3-21	0.0813	0.0084	1.1599	-3.4347	1.0000	0.0353	4.0768
PM3-22	0.0785	0.0085	1.1594	-3.4332	1.0000	0.0352	4.1021
PM3-23	0.0575	0.0084	1.1602	-3.4368	1.0000	0.0353	4.0975
PM3-24	0.0769	0.0079	1.1597	-3.4161	1.0000	0.0337	4.4582
PM3-25	0.0645	0.0084	1.1604	-3.4391	1.0000	0.0355	4.0556
PM3-26	0.0630	0.0078	1.1603	-3.4195	1.0000	0.0337	4.4421
PM3-27	0.0646	0.0083	1.1559	-3.4029	1.0000	0.0333	4.5789
PM3-28	0.0507	0.0082	1.1566	-3.4066	1.0000	0.0333	4.5643
PM3-29	0.0508	0.0072	1.1702	-3.4669	1.0000	0.0353	4.0613
PM3-30	0.0428	0.0071	1.1710	-3.4716	1.0000	0.0354	4.0338
Mean	0.0613	0.0079	1.1621	-3.4367	1.0000	0.0347	4.2154
SD	0.0241	0.0004	0.0055	0.0270	0.0000	0.0010	0.2232

$$\Delta H(T) = 0.0613(\pm 0.0241) + 0.0079(\pm 0.0004)T + 1.1621(\pm 0.0055) \cdot 10^{-4}T^2 - 3.4367(\pm 0.0270) \cdot 10^{-8}T^3$$

$$T \in [100K, 1000K]$$

$$\Delta a_0 = 0.1012 \text{kcal} \cdot \text{mol}^{-1}$$

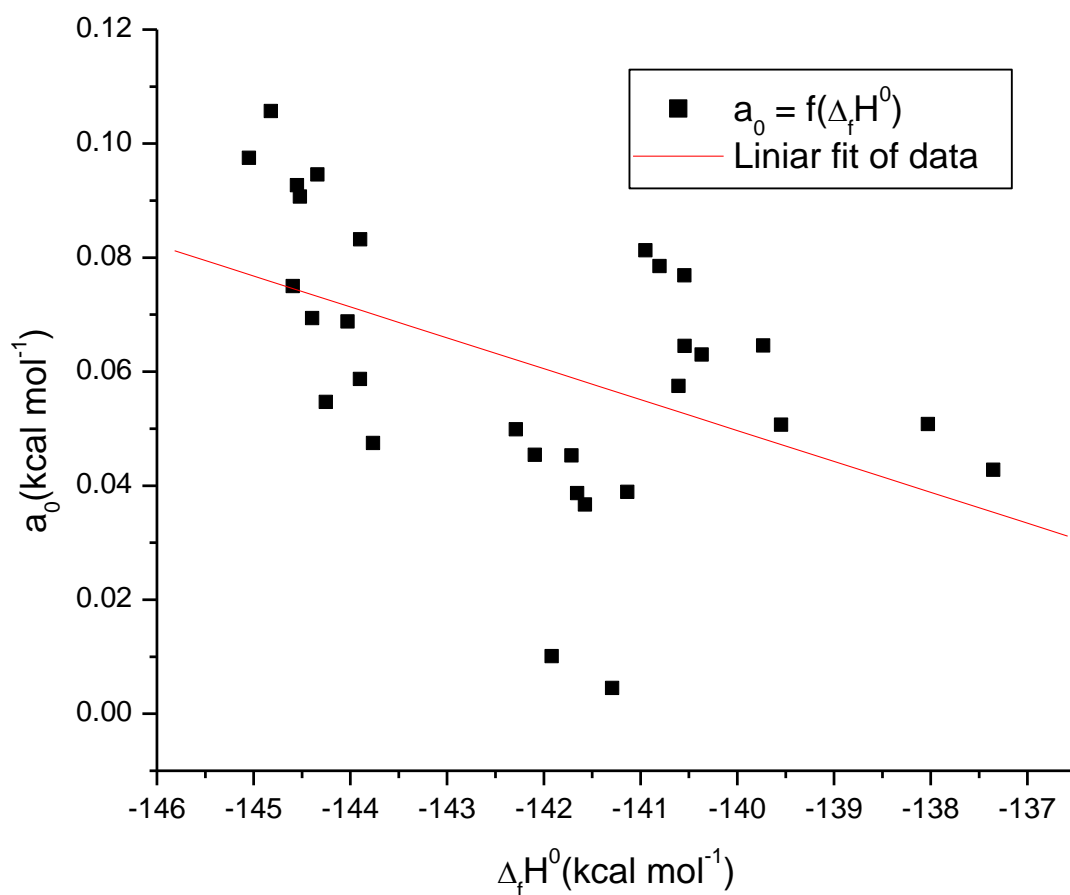


Fig. 2a. $\mathbf{a_0(PM3) = -0.7090 - 0.0054\Delta_f H^0(PM3)}$ ($r^2 = 0.1955$; $SD = 0.0217$; $F = 8.0474 > 1.0$)

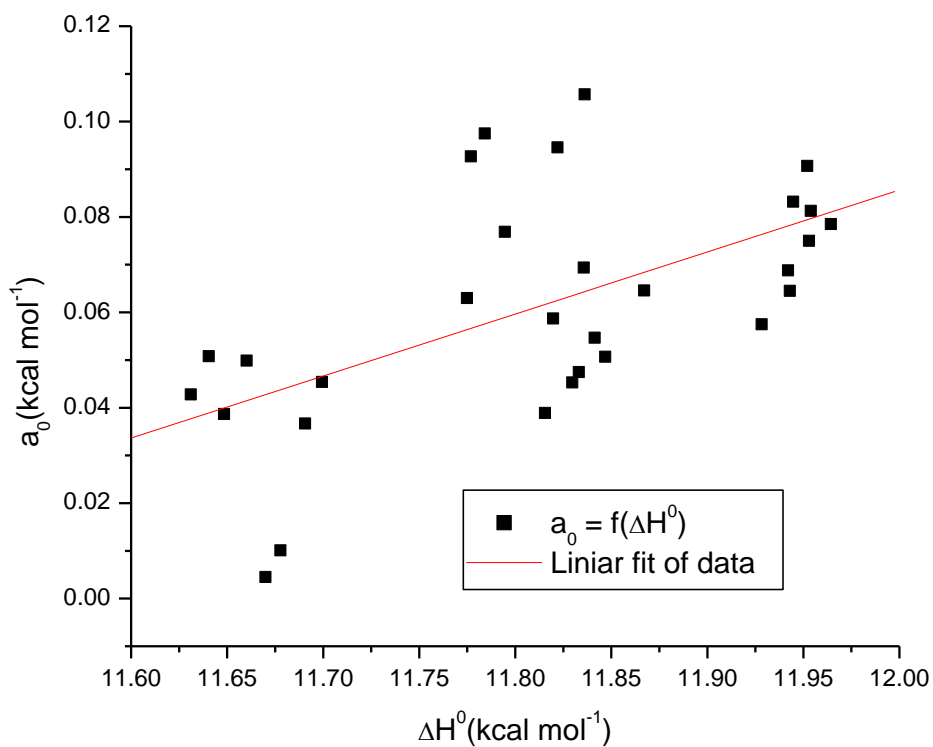


Fig. 2b. $\mathbf{a_0(PM3) = -1.4746 + 0.1300\Delta H^0(PM3)}$ ($r^2 = 0.3125$; $SD = 0.0200$; $F = 14.1835$)

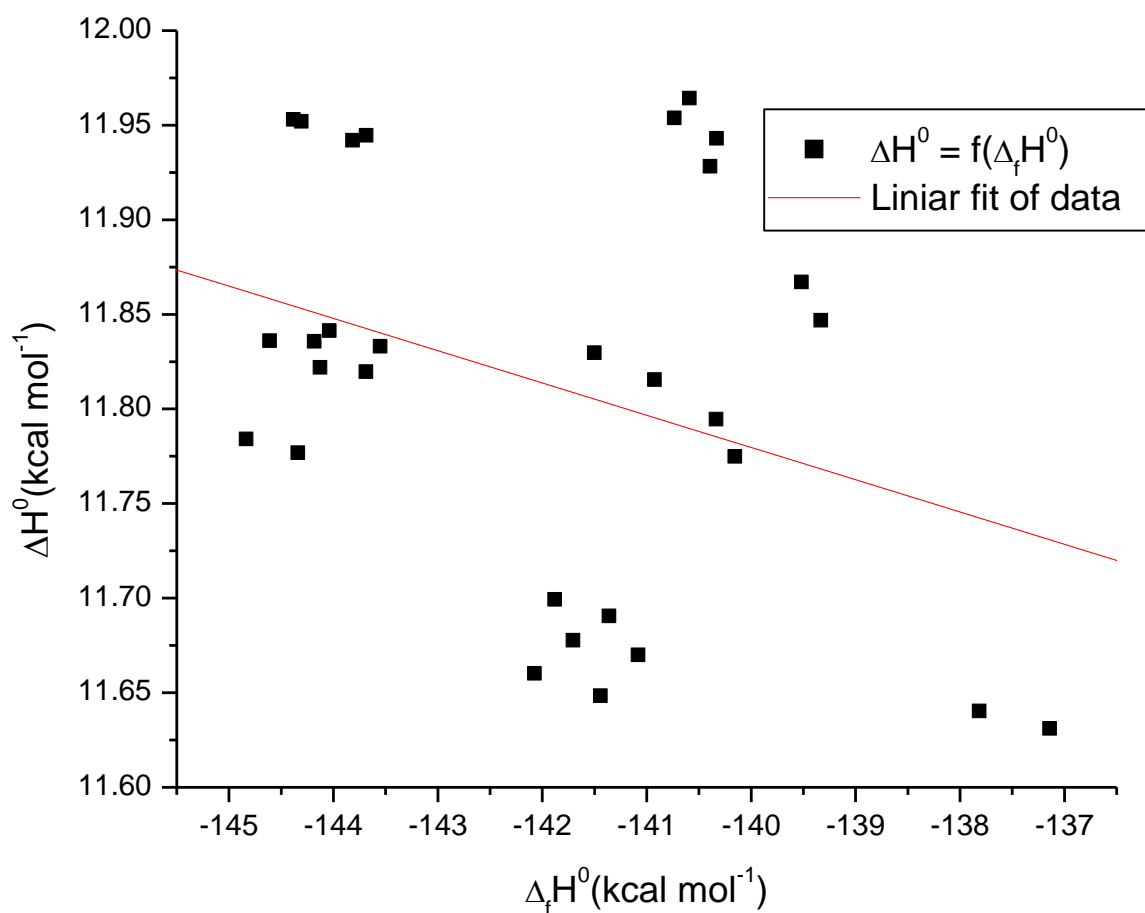


Fig. 2c. $\Delta H^0(\text{PM3}) = 9.3916 - 0.0171\Delta_r H^0(\text{PM3})$ ($r^2 = 0.0794$; $\text{SD} = 0.1033$; $F = 3.5033$)

Table 3a.
 $\Delta S(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ 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	89.1209	90.0290	89.8645	88.9819	90.3275	89.1576	89.5872	88.9456	89.7148	90.2077	88.7269	88.7595	86.7098	86.8610	86.2258
150	103.5423	104.5208	104.5722	103.3871	105.0108	103.6692	104.0595	103.4767	104.3990	104.8693	103.2146	103.2745	100.9240	101.2089	100.4700
200	116.4937	117.5108	117.7067	116.3329	118.1291	116.6992	117.0434	116.5235	117.5258	117.9837	116.2363	116.3171	113.7964	114.1380	113.3927
250	128.5627	129.6058	129.9061	128.4023	130.3185	128.8328	129.1386	128.6700	129.7246	130.1764	128.3687	128.4652	125.8441	126.1978	125.4872
298	139.6113	140.6721	141.0524	139.4531	141.4585	139.9354	140.2069	139.7814	140.8724	141.3212	139.4726	139.5798	136.8988	137.2448	136.5793
300	140.0626	141.1241	141.5075	139.9045	141.9133	140.3888	140.6590	140.2352	141.3275	141.7762	139.9262	140.0337	137.3508	137.6962	137.0326
350	151.1440	152.2186	152.6719	150.9883	153.0735	151.5206	151.7558	151.3728	152.4938	152.9409	151.0597	151.1746	148.4518	148.7815	148.1648
400	161.8637	162.9479	163.4614	161.7101	163.8600	162.2854	162.4868	162.1413	163.2846	163.7309	161.8260	161.9457	159.1958	159.5089	158.9339
450	172.2361	173.3272	173.8927	172.0839	174.2892	172.6976	172.8672	172.5556	173.7169	174.1627	172.2392	172.3621	169.5928	169.8908	169.3514
500	182.2618	183.3581	183.9684	182.1108	184.3633	182.7582	182.8989	182.6174	183.7932	184.2387	182.3005	182.4254	179.6418	179.9270	179.4171
550	191.9417	193.0419	193.6907	191.7914	194.0843	192.4683	192.5832	192.3281	193.5158	193.9610	192.0111	192.1372	189.3428	189.6173	189.1320
600	201.2804	202.3836	203.0652	201.1308	203.4579	201.8330	201.9252	201.6931	202.8906	203.3357	201.3761	201.5030	198.7003	198.9661	198.5012
650	210.2870	211.3926	212.1022	210.1379	212.4942	210.8619	210.9344	210.7221	211.9278	212.3728	210.4053	210.5327	207.7234	207.9822	207.5342
700	218.9737	220.0811	220.8147	218.8251	221.2060	219.5677	219.6231	219.4279	220.6404	221.0853	219.1113	219.2391	216.4246	216.6777	216.2439
750	227.3546	228.4634	229.2175	227.2064	229.6083	227.9650	228.0055	227.8251	229.0434	229.4881	227.5087	227.6368	224.8183	225.0666	224.6448
800	235.4446	236.5545	237.3261	235.2968	237.7165	236.069	236.0968	235.9291	237.1522	237.5969	235.6130	235.7411	232.9195	233.1640	232.7523
850	243.2588	244.3695	245.1562	243.1113	245.5462	243.8953	243.9120	243.7552	244.9824	245.4271	243.4394	243.5676	240.7435	240.9849	240.5819
900	250.8117	251.9232	252.7228	250.6646	253.1125	251.4587	251.4658	251.3185	252.5492	252.9938	251.0029	251.1312	248.3051	248.5440	248.1485
950	258.1176	259.2295	260.0403	257.9707	260.4298	258.7735	258.7723	258.6332	259.8670	260.3115	258.3179	258.4463	255.6187	255.8554	255.4663
1000	265.1895	266.3019	267.1224	265.0430	267.5117	265.8533	265.8448	265.7129	266.9492	267.3936	265.3979	265.5262	262.6975	262.9325	262.5490

Table 3b.
 $\Delta S(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ 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	87.7850	86.3841	86.6338	86.0630	87.5167	89.6179	89.7545	88.8928	88.1990	89.1969	87.6808	88.9552	88.4433	86.1379	85.9418
150	102.3112	100.5781	100.9633	100.2895	102.0184	104.3213	104.4661	103.5616	102.6731	103.8788	102.1275	103.5164	102.9753	100.4137	100.1956
200	115.3552	113.4466	113.8888	113.2070	115.0522	117.4485	117.6052	116.6833	115.6604	117.0069	115.1055	116.5778	116.0269	113.2926	113.0695
250	127.5105	125.4969	125.9515	125.3025	127.2045	129.6494	129.8162	128.8871	127.7545	129.2161	127.1983	128.7294	128.1771	125.3155	125.0947
298	138.6401	136.5559	137.0027	136.3973	138.3338	140.8048	140.9788	140.0463	138.8230	140.3803	138.2678	139.8382	139.2871	136.3406	136.1240
300	139.0948	137.0080	137.4543	136.8508	138.7885	141.2603	141.4346	140.5020	139.2751	140.8362	138.7200	140.2917	139.7407	136.7913	136.5749
350	150.2571	148.1131	148.5440	147.9860	149.9512	152.4388	152.6186	151.6833	150.3753	152.0224	149.8215	151.4218	150.8722	147.8662	147.6540
400	161.0516	158.8603	159.2748	158.7576	160.7461	163.2436	163.4273	162.4896	161.1129	162.8330	160.5598	162.1808	161.6320	158.5909	158.3822
450	171.4911	169.2597	169.6595	169.1769	171.1857	173.6895	173.8763	172.9363	171.5021	173.2834	170.9492	172.5856	172.0371	168.9746	168.7687
500	181.5759	179.3106	179.6977	179.2441	181.2705	183.7785	183.9678	183.0255	181.5437	183.3757	180.9907	182.6388	182.0902	179.0148	178.8110
550	191.3072	189.0129	189.3896	188.9600	191.0017	193.5123	193.7036	192.7594	191.2385	193.1121	190.6851	192.3423	191.7934	188.7100	188.5078
600	200.6904	198.3715	198.7396	198.3300	200.3847	202.8969	203.0900	202.1439	200.5911	202.4987	200.0374	201.7017	201.1524	198.0638	197.8628
650	209.7353	207.3955	207.7567	207.3638	209.4295	211.9425	212.1370	211.1895	209.6108	211.5459	209.0566	210.7266	210.1768	207.0846	206.8847
700	218.4550	216.0975	216.4531	216.0740	218.1491	220.6623	220.8582	219.9093	218.3096	220.2671	217.7550	219.4295	218.8794	215.7843	215.5853
750	226.8643	224.4918	224.8429	224.4755	226.5583	229.0713	229.2684	228.3185	226.7017	228.6773	226.1468	227.8249	227.2745	224.1770	223.9788
800	234.9789	232.5936	232.9409	232.5835	234.6729	237.1853	237.3835	236.4327	234.8021	236.7923	234.2469	235.9280	235.3773	232.2776	232.0801
850	242.8144	240.4181	240.7625	240.4135	242.5084	245.0200	245.2191	244.2676	242.6258	244.6279	242.0704	243.7540	243.2030	240.1013	239.9044
900	250.3859	247.9803	248.3222	247.9805	250.0799	252.5906	252.7906	251.8385	250.1877	252.1993	249.6320	251.3176	250.7665	247.6628	247.4665
950	257.7079	255.2943	255.6341	255.2987	257.4020	259.9116	260.1124	259.1598	257.5017	259.5210	256.9459	258.6331	258.0819	254.9763	254.7805
1000	264.7941	262.3735	262.7116	262.3817	264.4882	266.9966	267.1982	266.2452	264.5812	266.6067	264.0252	265.7139	265.1625	262.0550	261.8599

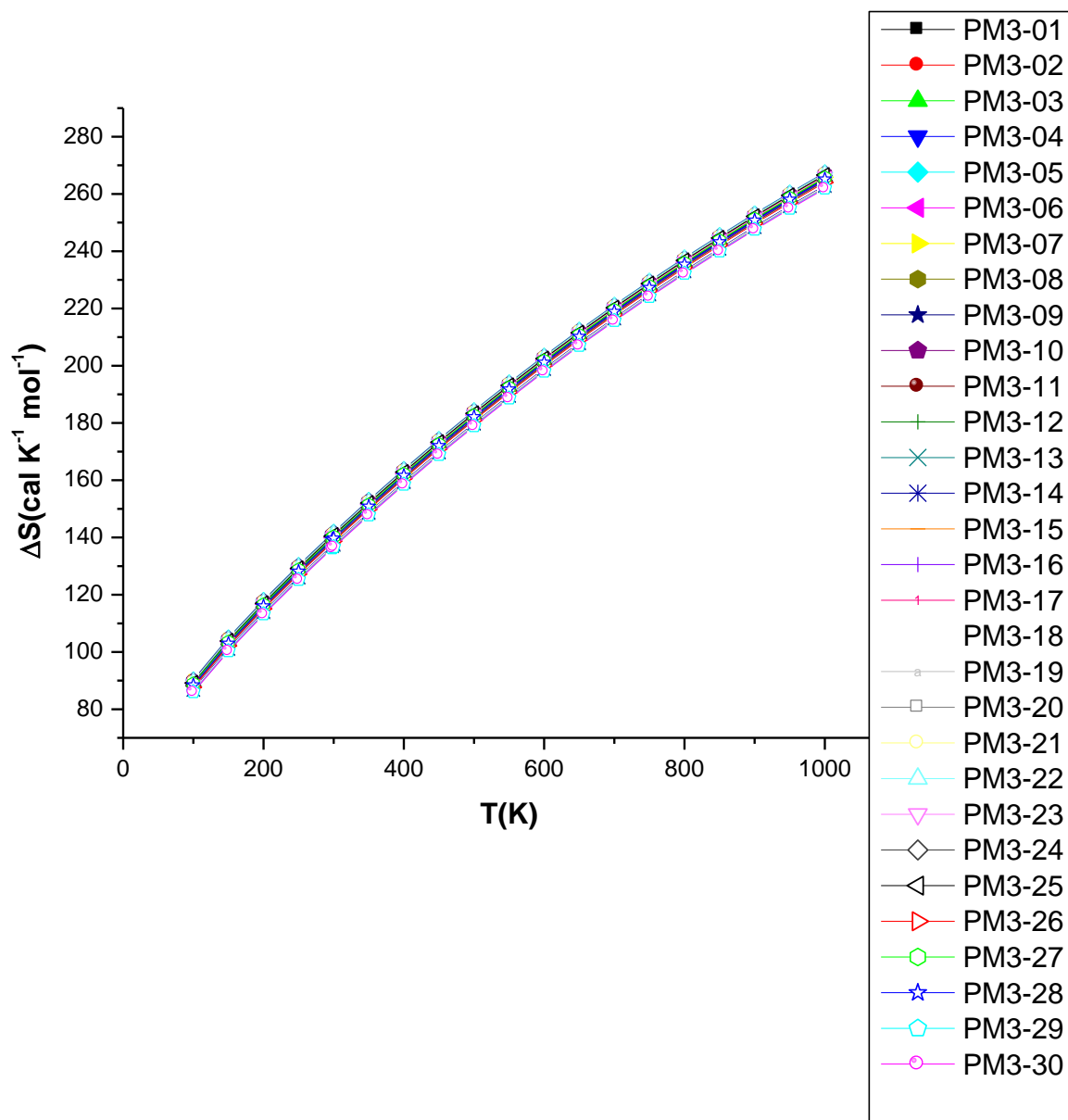


Fig. 3. Functional dependencies $\Delta S(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$ graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM3-M12

Table 4.

M12 Polynomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of $\Delta S(\text{cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1})$ (T) for distinct conformers energetic and geometric optimization with by PM3-M12 of (3R,5S,6R)-6-acetylamidopenicillanic acid

Conformer	a_0	a_1	$a_2\cdot 10^4$	$a_3\cdot 10^8$	r^2	SD	$F\cdot 10^{-5}$
PM3-01	61.4035	0.2965	-1.2467	3.2223	1.0000	0.2969	2.10143
PM3-02	62.2187	0.2978	-1.2654	3.3109	1.0000	0.3046	1.99942
PM3-03	61.7219	0.3020	-1.3160	3.5267	1.0000	0.3229	1.79747
PM3-04	61.2680	0.2963	-1.2436	3.2045	1.0000	0.2933	2.15396
PM3-05	62.2206	0.3015	-1.3087	3.4917	1.0000	0.3199	1.82934
PM3-06	61.2519	0.2986	-1.2670	3.2930	1.0000	0.2994	2.08041
PM3-07	61.7812	0.2976	-1.2620	3.2916	1.0000	0.3005	2.05497
PM3-08	60.9959	0.2991	-1.2749	3.3306	1.0000	0.3008	2.06329
PM3-09	61.5801	0.3018	-1.3117	3.5032	1.0000	0.3182	1.85057
PM3-10	62.0972	0.3014	-1.3056	3.4724	1.0000	0.3148	1.89041
PM3-11	60.8305	0.2983	-1.2623	3.2676	1.0000	0.2947	2.14755
PM3-12	60.8096	0.2990	-1.2721	3.3139	1.0000	0.2969	2.11748
PM3-13	59.1288	0.2937	-1.1907	2.9163	1.0000	0.2579	2.78952
PM3-14	59.2030	0.2954	-1.2253	3.1089	1.0000	0.2854	2.27661
PM3-15	58.5095	0.2950	-1.2055	2.9726	1.0000	0.2544	2.87894
PM3-16	59.8283	0.2990	-1.2631	3.2524	1.0000	0.2940	2.16646
PM3-17	58.8009	0.2935	-1.1876	2.8975	1.0000	0.2532	2.89560
PM3-18	58.9730	0.2953	-1.2224	3.0908	1.0000	0.2809	2.35083
PM3-19	58.3489	0.2949	-1.2022	2.9537	1.0000	0.2504	2.97244
PM3-20	59.5748	0.2987	-1.2579	3.2255	1.0000	0.2896	2.23284
PM3-21	61.4807	0.3018	-1.3073	3.4714	1.0000	0.3185	1.85088
PM3-22	61.5872	0.3021	-1.3115	3.4898	1.0000	0.3184	1.85322
PM3-23	60.7557	0.3016	-1.3032	3.4486	1.0000	0.3117	1.93253
PM3-24	60.4106	0.2974	-1.2558	3.2605	1.0000	0.3020	2.03683
PM3-25	61.0420	0.3018	-1.3055	3.4570	1.0000	0.3124	1.92430
PM3-26	59.9024	0.2971	-1.2511	3.2349	1.0000	0.2968	2.10937
PM3-27	60.9794	0.2997	-1.2872	3.4035	1.0000	0.3078	1.96838
PM3-28	60.4780	0.2994	-1.2821	3.3763	1.0000	0.3022	2.04196
PM3-29	58.6140	0.2936	-1.1957	2.9608	1.0000	0.2779	2.39847
PM3-30	58.4175	0.2935	-1.1920	2.9387	1.0000	0.2728	2.48975
Mean	60.4738	0.2981	-1.2594	3.2563	1.0000	0.2950	2.17517
SD	1.2434	0.0029	0.0411	0.1969	0.0000	0.0206	0.33015

$$\Delta S(T) = 60.4738(\pm 1.2434) + 0.2981(\pm 0.0029)T - 1.2594(\pm 0.0411)\cdot 10^{-4}T^2 + 3.2563(\pm 0.1969)\cdot 10^{-8}T^3$$

$$T \in [100\text{K}, 1000\text{K}]$$

$$\Delta a_0 = 3.8031 \text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

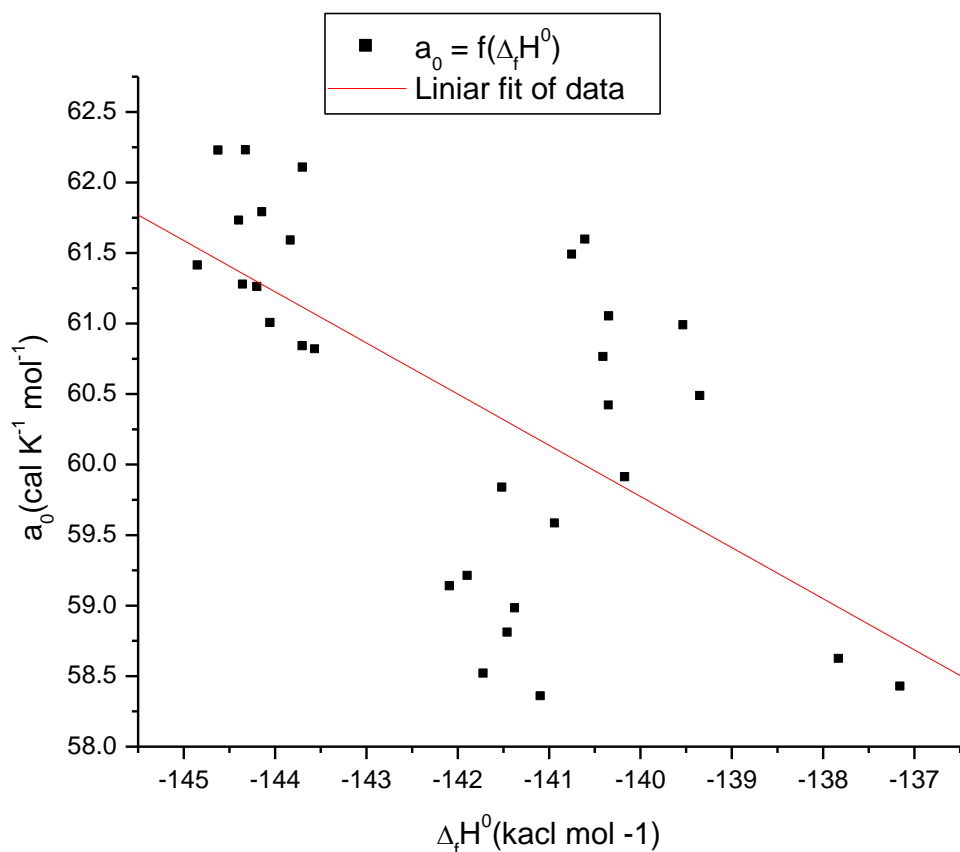


Fig. 4a. $a_0(\text{PM3}) = 8.9892 - 0.3627\Delta_f H^0(\text{PM3})$ ($r^2 = 0.3552$; $SD = 0.9985$; $F = 16.97 > 1$)

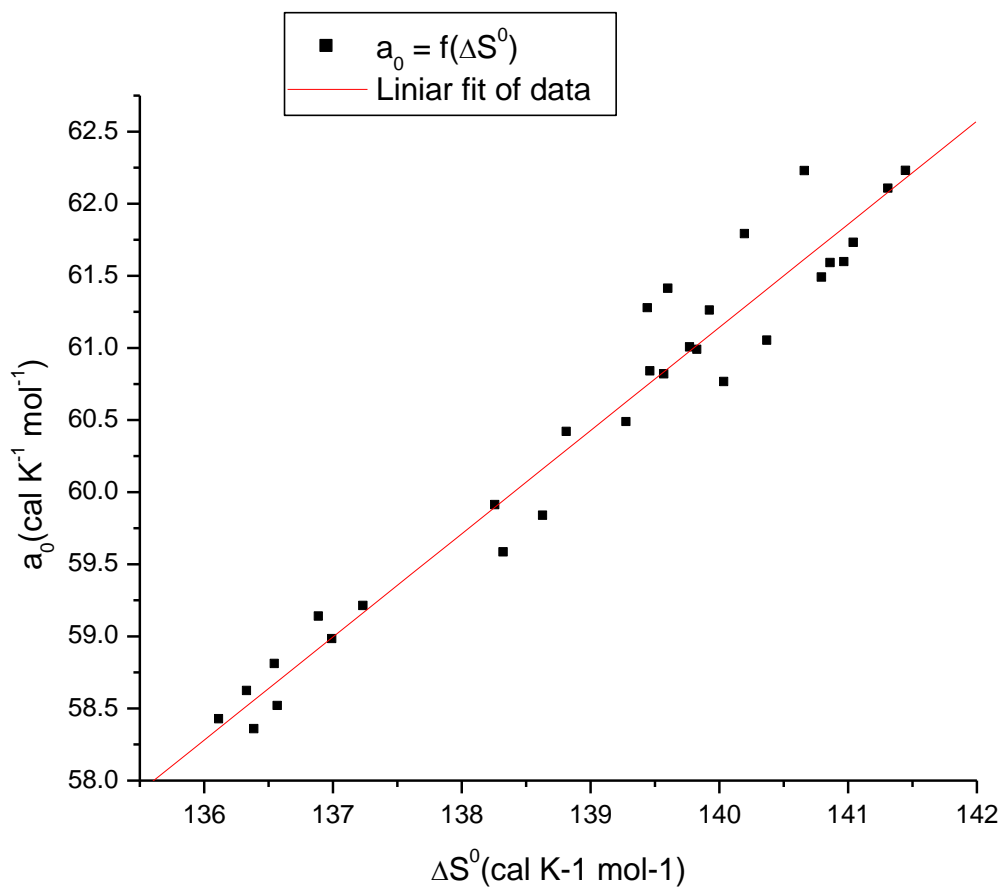


Fig. 4b. $a_0(\text{PM3}) = -39.0198 + 0.7155\Delta S^0(\text{PM3})$ ($r^2 = 0.9508$; $SD = 0.2759$; $F = 560.979$)

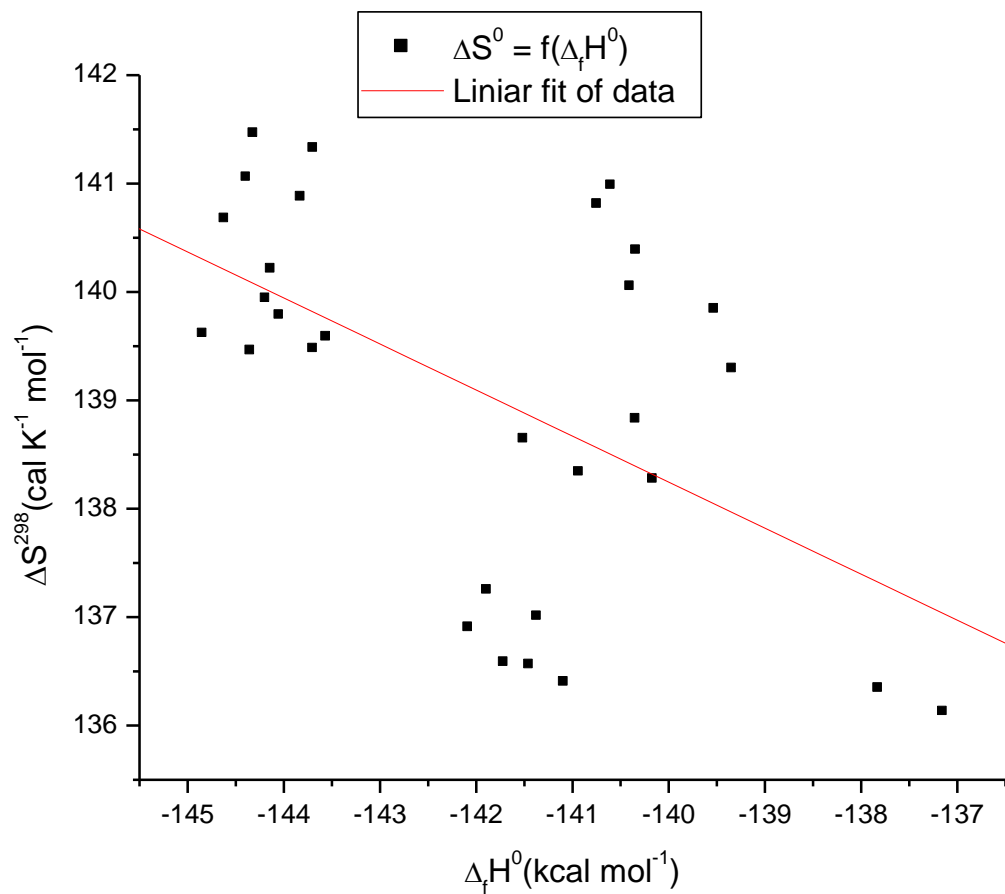


Fig. 4c. $\Delta S^0(\text{PM3}) = 78.7983 - 0.42462\Delta_r H^0(\text{PM3})$ ($r^2 = 0.2521$; SD = 1.4668; F = 10.78)

Table 5a.
 $C_p(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ 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	30.9826	31.1866	31.7115	30.9386	31.6592	31.1432	31.1274	31.1804	31.6409	31.5890	31.0729	31.1324	30.3340	30.6954	30.3344
150	40.6629	40.8097	41.3324	40.6322	41.2715	40.9256	40.7758	40.9812	41.2913	41.2397	40.8823	40.9540	40.2894	40.5581	40.4305
200	49.7626	49.8863	50.3674	49.7555	50.3167	50.0442	49.8783	50.1042	50.3551	50.3209	50.0295	50.1025	49.5886	49.7066	49.7895
250	58.7415	58.8499	59.3084	58.7503	59.2685	59.0397	58.8579	59.0946	59.3131	59.2920	59.0431	59.1092	58.7220	58.7165	58.9363
298	67.2998	67.3934	67.8472	67.3150	67.8157	67.6175	67.4073	67.6621	67.8582	67.8452	67.6281	67.6829	67.3867	67.3077	67.5953
300	67.6524	67.7454	68.1992	67.6678	68.1680	67.9709	67.7594	68.0150	68.2103	68.1975	67.9817	68.0359	67.7429	67.6617	67.9511
350	76.2717	76.3498	76.8027	76.2876	76.7782	76.6056	76.3637	76.6379	76.8141	76.8063	76.6173	76.6589	76.4320	76.3146	76.6272
400	84.3634	84.4283	84.8756	84.3774	84.8558	84.7032	84.4396	84.7253	84.8848	84.8798	84.7131	84.7438	84.5629	84.4343	84.7433
450	91.7923	91.8461	92.2804	91.8038	92.2640	92.1283	91.8546	92.1426	92.2870	92.2836	92.1359	92.1580	92.0099	91.8837	92.1757
500	98.5239	98.5687	98.9835	98.5334	98.9696	98.8486	98.5748	98.8572	98.9881	98.9856	98.8542	98.8700	98.7464	98.6291	98.8985
550	104.5893	104.6267	105.0174	104.597	105.0055	104.8975	104.6311	104.9022	105.0207	105.0186	104.9016	104.9128	104.8085	104.7027	104.9482
600	110.0503	110.0816	110.4458	110.0572	110.4355	110.3391	110.0849	110.3411	110.4484	110.4466	110.3423	110.3503	110.2617	110.1678	110.3902
650	114.9776	115.0040	115.3408	114.9839	115.3318	115.2457	115.0067	115.2461	115.3431	115.3415	115.2485	115.2541	115.1789	115.0963	115.2975
700	119.4389	119.4611	119.7709	119.4449	119.7630	119.6863	119.4636	119.6856	119.7732	119.7717	119.6889	119.6928	119.6291	119.5568	119.7389
750	123.4940	123.5127	123.7965	123.4998	123.7896	123.7213	123.5151	123.7198	123.7990	123.7977	123.7238	123.7265	123.6729	123.6098	123.7747
800	127.1935	127.2092	127.4686	127.1993	127.4626	127.4018	127.2117	127.3999	127.4714	127.4702	127.4044	127.4062	127.3613	127.3064	127.4561
850	130.5798	130.5930	130.8297	130.5856	130.8245	130.7703	130.5955	130.7683	130.8329	130.8318	130.7731	130.7742	130.7370	130.6891	130.8255
900	133.6880	133.6991	133.9151	133.6939	133.9105	133.8623	133.7018	133.8602	133.9186	133.9176	133.8653	133.8659	133.8354	133.7936	133.918
950	136.5479	136.5571	136.7542	136.5538	136.7502	136.7074	136.5600	136.7052	136.7580	136.7571	136.7105	136.7107	136.6859	136.6495	136.7635
1000	139.1844	139.1920	139.3719	139.1903	139.3685	139.3304	139.1950	139.3282	139.3760	139.3752	139.3337	139.3335	139.3138	139.2819	139.3867

Table 5b.
 $C_p(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ computed by PM3-M12

Conf	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
T(K)															
100	31.1804	30.2678	30.6363	30.2824	31.1115	31.7236	31.7279	31.5972	31.0930	31.6439	31.0107	31.2847	31.1961	30.4921	30.4231
150	40.9613	40.2594	40.5305	40.3996	40.9135	41.3046	41.3398	41.2604	40.7962	41.2837	40.7475	41.0395	40.9881	40.3886	40.3539
200	50.1141	49.5908	49.7095	49.7847	50.0917	50.3533	50.3986	50.3558	49.8788	50.3783	49.8626	50.1431	50.1263	49.5304	49.5298
250	59.1681	58.7421	58.7373	58.9483	59.1625	59.3390	59.3825	59.3591	58.8525	59.3856	58.8550	59.0979	59.1009	58.5686	58.5881
298	67.7960	67.4129	67.3350	67.6140	67.7975	67.9205	67.9588	67.9417	67.4168	67.9719	67.4251	67.6293	67.6384	67.2103	67.2373
300	68.1511	67.7691	67.6892	67.9699	68.1528	68.2740	68.3121	68.2951	67.7698	68.3253	67.7781	67.9808	67.9900	67.5666	67.5937
350	76.8191	76.4577	76.3420	76.6467	76.8222	76.9079	76.9405	76.9233	76.3997	76.9555	76.4069	76.5756	76.5835	76.2729	76.3004
400	84.9323	84.5853	84.4588	84.7607	84.9344	84.9967	85.0247	85.0056	84.5020	85.0377	84.5056	84.6472	84.6514	84.4347	84.4595
450	92.3604	92.0287	91.9048	92.1904	92.3609	92.4066	92.4312	92.4105	91.9396	92.4411	91.9397	92.0598	92.0602	91.9129	91.9342
500	99.0757	98.7621	98.6471	98.9108	99.0749	99.1079	99.1301	99.1088	98.6780	99.1369	98.6754	98.7780	98.7756	98.6755	98.6937
550	105.1151	104.8218	104.7182	104.9586	105.1136	105.1362	105.1567	105.1358	104.7480	105.1610	104.7438	104.8318	104.8278	104.7579	104.7736
600	110.5449	110.2734	110.1815	110.3994	110.5432	110.5571	110.5763	110.5566	110.2119	110.5786	110.2068	110.2827	110.2779	110.2262	110.2401
650	115.4391	115.1895	115.1087	115.3058	115.4374	115.4437	115.4621	115.4439	115.1406	115.4630	115.1353	115.2009	115.1958	115.1544	115.1671
700	119.8672	119.6390	119.5684	119.7466	119.8658	119.8656	119.8832	119.8667	119.6020	119.8831	119.5968	119.6536	119.6487	119.6125	119.6243
750	123.8902	123.6822	123.6208	123.7822	123.8893	123.8833	123.9002	123.8856	123.6560	123.8995	123.6511	123.7005	123.6960	123.6619	123.6732
800	127.5594	127.3704	127.3168	127.4634	127.5590	127.5481	127.5644	127.5515	127.3534	127.5633	127.3490	127.3920	127.3880	127.3544	127.3652
850	130.9174	130.7459	130.6993	130.8326	130.9175	130.9024	130.9182	130.9070	130.7368	130.9168	130.7329	130.7704	130.7670	130.7330	130.7435
900	133.9997	133.8440	133.8035	133.9252	134.0003	133.9817	133.9970	133.9872	133.8416	133.9954	133.8382	133.8709	133.8681	133.8334	133.8436
950	136.8358	136.6945	136.6591	136.7705	136.8368	136.8153	136.8300	136.8216	136.6974	136.8285	136.6945	136.7232	136.7210	136.6854	136.6954
1000	139.4506	139.3222	139.2913	139.3936	139.4520	139.4281	139.4423	139.4351	139.3295	139.4408	139.3271	139.3522	139.3505	139.3143	139.3241

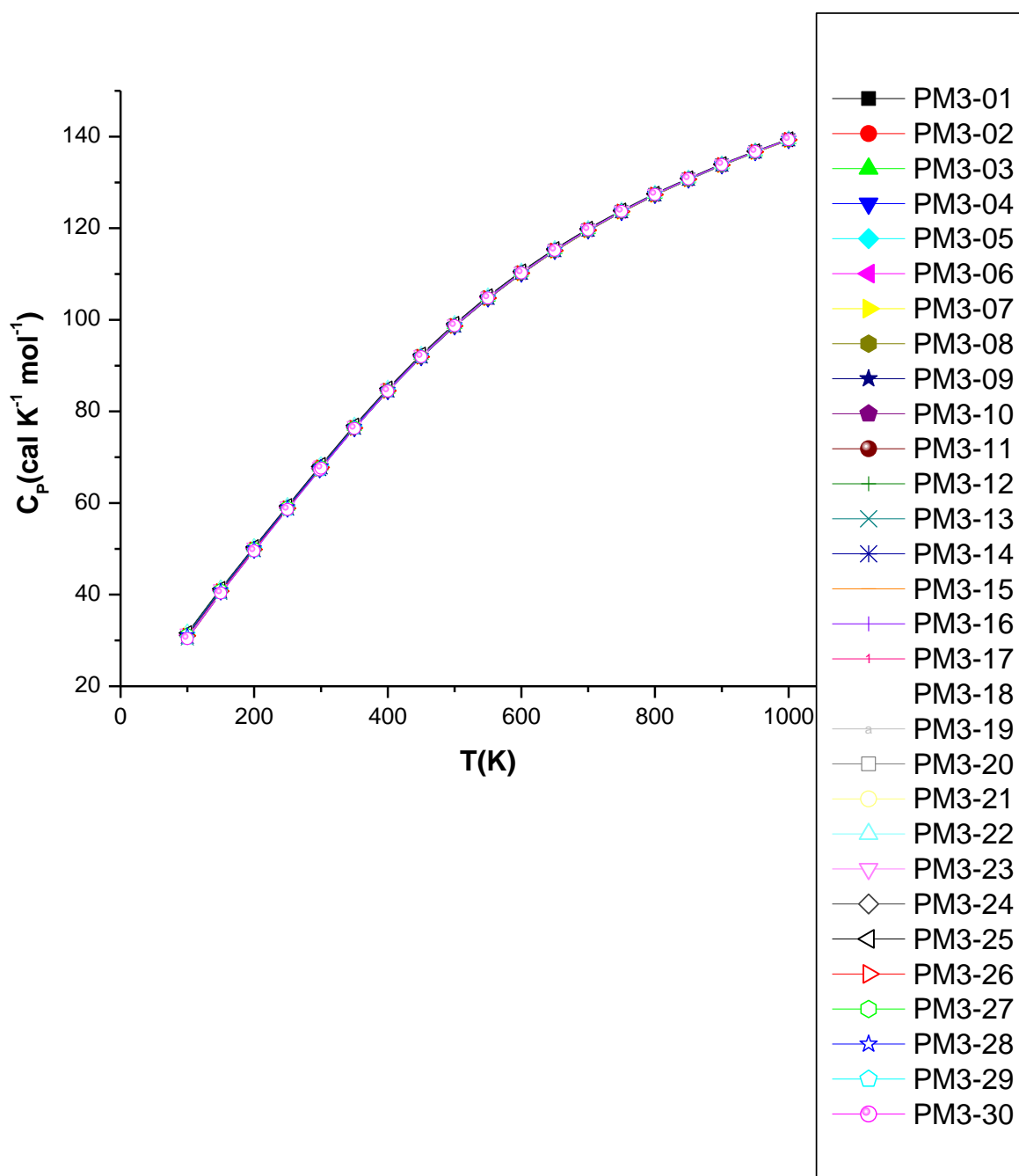


Fig. 5. Functional dependencies $C_P(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$ graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM3-M12

Table 6.

M12 Polinomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of $C_p(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ for distinct conformers energetic and geometric optimization with by PM3-M12 of (3R,5S,6R)-6-acetylamidopenicillanic acid

Conformer	a_0	a_1	$a_2\cdot 10^4$	$a_3\cdot 10^8$	r^2	SD	F
PM3-01	7.9031	0.2342	-1.1379	1.0253	0.9998	0.5406	25110.6
PM3-02	8.1661	0.2334	-1.1281	0.9839	0.9997	0.5434	24772.2
PM3-03	8.6953	0.2333	-1.13156	0.9942	0.9997	0.5553	23575.8
PM3-04	7.8121	0.2348	-1.1482	1.0792	0.9998	0.5357	25577.1
PM3-05	8.6136	0.2335	-1.1337	1.0011	0.9997	0.5569	23465.2
PM3-06	7.9377	0.2360	-1.1688	1.1696	0.9998	0.5395	25163.9
PM3-07	8.0569	0.2341	-1.1403	1.0485	0.9998	0.5369	25386.5
PM3-08	7.9893	0.2360	-1.1726	1.1983	0.9997	0.5327	25785.1
PM3-09	8.5708	0.2340	-1.1448	1.0636	0.9997	0.5481	24210.9
PM3-10	8.4788	0.2344	-1.1506	1.0908	0.9997	0.5475	24291.8
PM3-11	7.8109	0.2367	-1.1820	1.2386	0.9998	0.5329	25811.5
PM3-12	7.8906	0.2367	-1.1845	1.2611	0.9998	0.5267	26373.3
PM3-13	6.6983	0.2412	-1.2451	1.5345	0.9998	0.5158	27847.4
PM3-14	7.4609	0.2366	-1.1704	1.1679	0.9998	0.5325	26007.9
PM3-15	6.6072	0.2431	-1.2823	1.7369	0.9998	0.4919	30585.1
PM3-16	7.7788	0.2378	1.1962	1.2883	0.9997	0.5483	24399.0
PM3-17	6.5724	0.2421	-1.2604	1.6158	0.9998	0.5074	28794.0
PM3-18	7.3430	0.2374	-1.1850	1.2450	0.9998	0.5250	26774.7
PM3-19	6.5030	0.2438	-1.2944	1.7999	0.9997	0.4860	31341.2
PM3-20	7.6594	0.2384	-1.2074	1.3466	0.9997	0.5428	24915.7
PM3-21	8.5673	0.2343	-1.1453	1.0449	0.9997	0.5690	22486.0
PM3-22	8.5683	0.2346	-1.1510	1.0782	0.9997	0.5628	22974.4
PM3-23	8.3759	0.2355	-1.1674	1.1648	0.9997	0.5521	23900.3
PM3-24	8.0223	0.2341	-1.1332	0.9888	0.9997	0.5453	24697.4
PM3-25	8.4102	0.2355	-1.1676	1.1645	0.9997	0.5555	23598.2
PM3-26	7.8822	0.2350	-1.1480	1.0679	0.9998	0.5366	25520.5
PM3-27	8.2454	0.2344	-1.1475	1.0874	0.9998	0.5260	26420.9
PM3-28	8.0954	0.2353	-1.1634	1.1722	0.9998	0.5166	27408.9
PM3-29	7.1342	0.2376	-1.1768	1.1631	0.9997	0.5526	24267.1
PM3-30	6.9993	0.2385	-1.1929	1.2475	0.9997	0.5445	25017.8
Mean	7.8283	0.2364	-1.0955	1.2023	0.99975	0.536	25549.35
SD	0.6499	0.0029	0.4350	0.2133	0.00005	0.0191	2042.21

$$C_p(T) = 7.8283(\pm 0.6499) + 0.2364(\pm 0.0029)T - 1.0955(\pm 0.4350)\cdot 10^{-4}T^2 + 1.2023(\pm 0.2133)\cdot 10^{-8}T^3$$

$$T \in [100\text{K}, 1000\text{K}] \text{ (SD = } \mathbf{0.5360} \pm 0.0191; \mathbf{25549.35} (\pm 2042.21))$$

$$\Delta a_0 = 2.1923 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

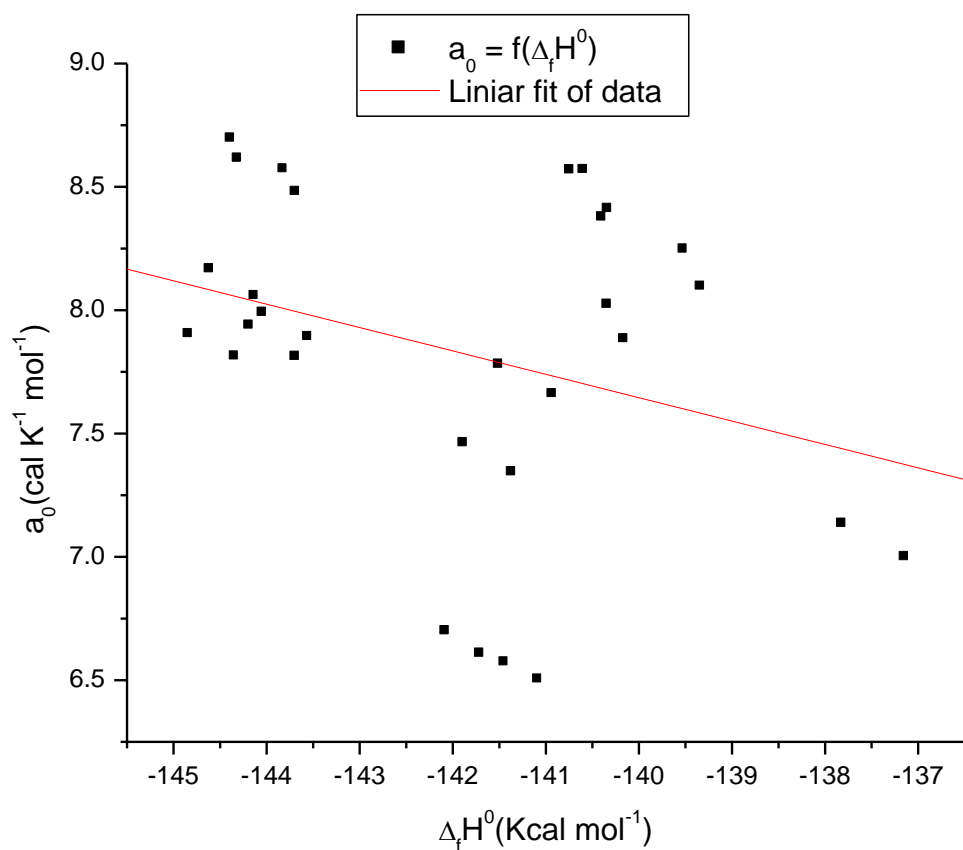


Fig. 6a. $a_0(\text{PM3}) = -5.6212 - 0.0947\Delta_f H^0(\text{PM3})$ ($r^2 = 0.0619$; $F = 2.91$)

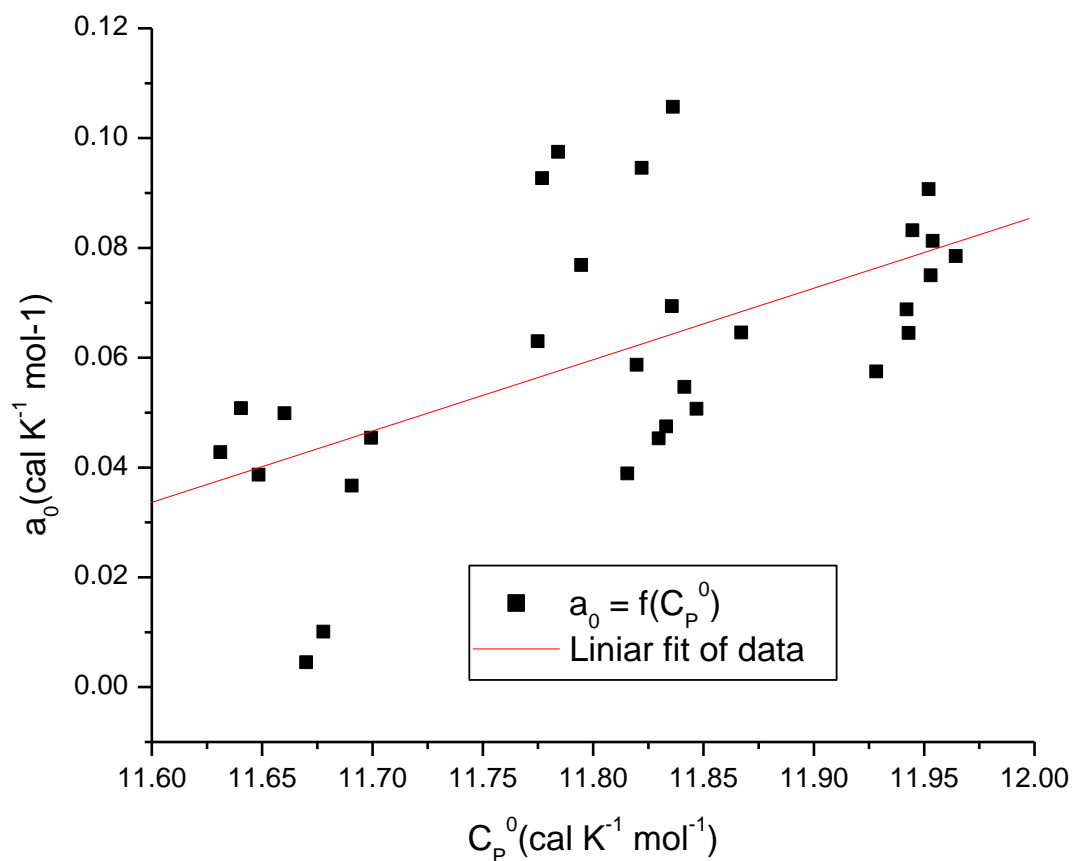


Fig. 6b. $a_0(\text{PM3}) = -1.4746 + 0.1300C_p^0(\text{PM3})$ ($r^2 = 0.3125$; $\text{SD} = 0.0200$ $F = 14.1834$)

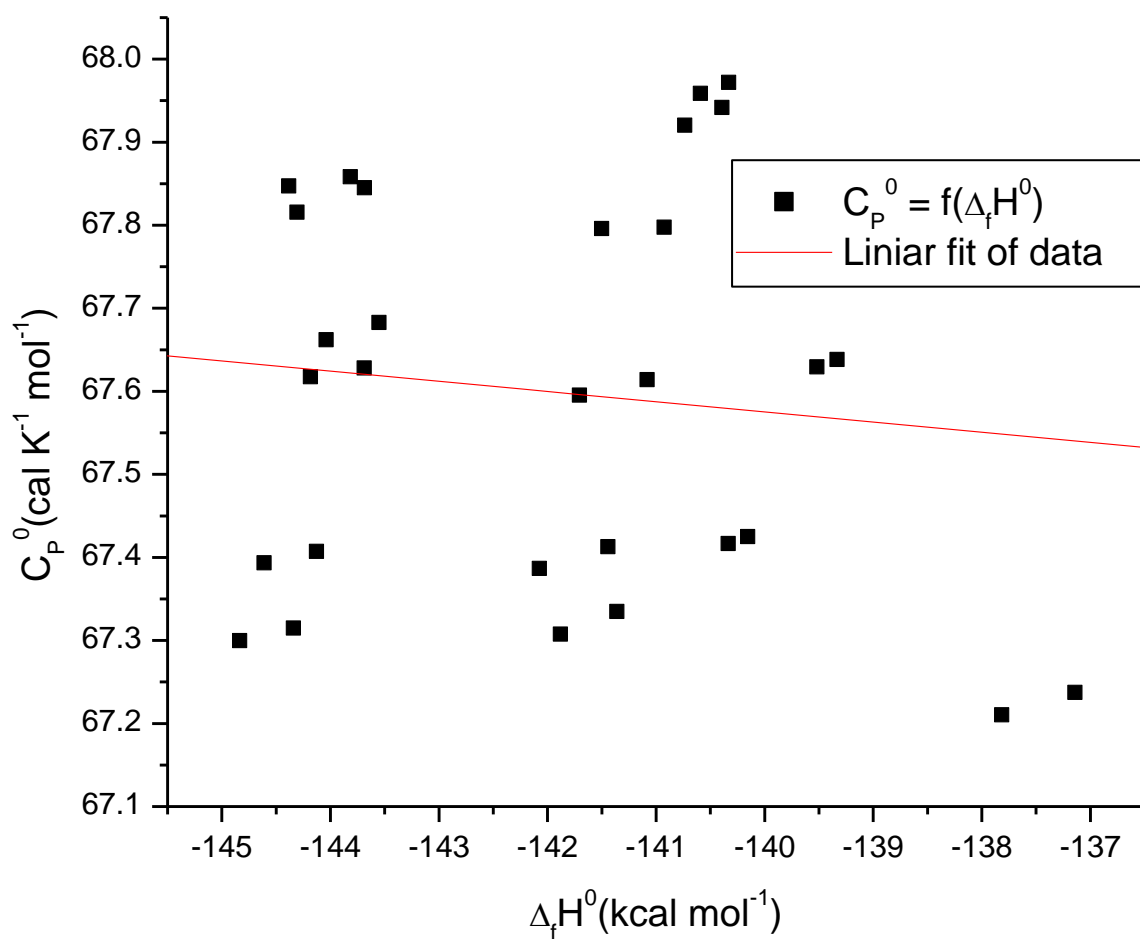


Fig. 6c. $C_p^0(\text{PM3}) = 65.8593 - 0.0123\Delta_f H^0(\text{PM3})$ ($r^2 = 0.0117$; $\text{SD} = 0.2411$; $F = 0.3322$)

Table 7.
 $\Delta H(\text{kcal}\cdot\text{mol}^{-1}) = f(T)$ computed by PM6-M12

Conf	PM6-01	PM6-02	PM6-03	PM6-04	PM6-05	PM6-06	PM6-07	PM6-08
T(K)								
100	2.0908	2.086	2.0853	1.9878	2.0759	1.981	2.0746	2.0622
150	3.9725	3.9667	3.9466	3.8168	3.9372	3.8079	3.9426	3.9308
200	6.3188	6.3129	6.2745	6.124	6.2659	6.1141	6.2783	6.268
250	9.1109	9.1055	9.0529	8.8888	9.0457	8.8788	9.0626	9.0544
298	12.2124	12.2074	12.1451	11.9726	12.1391	11.9624	12.1587	12.1524
300	12.3506	12.3455	12.2829	12.1102	12.277	12.0999	12.2966	12.2905
350	16.034	16.029	15.9593	15.7813	15.9542	15.7705	15.976	15.9714
400	20.1431	20.1376	20.063	19.8818	20.0581	19.8701	20.082	20.0785
450	24.6491	24.6428	24.5644	24.3817	24.5595	24.3687	24.5854	24.5826
500	29.5185	29.5112	29.4299	29.2465	29.4247	29.2322	29.4527	29.4503
550	34.7178	34.7095	34.6258	34.4424	34.6201	34.4265	34.6503	34.648
600	40.2156	40.2062	40.1204	39.9374	40.1142	39.9202	40.1466	40.1444
650	45.9834	45.9729	45.8854	45.7031	45.8785	45.6844	45.9132	45.911
700	51.9957	51.9841	51.8951	51.7137	51.8876	51.6937	51.9245	51.9223
750	58.2298	58.2172	58.1268	57.9464	58.1187	57.9252	58.1579	58.1557
800	64.6654	64.6519	64.5603	64.3811	64.5516	64.3587	64.5932	64.5908
850	71.2846	71.2702	71.1775	70.9995	71.1683	70.976	71.2121	71.2096
900	78.0711	78.0559	77.9622	77.7854	77.9524	77.7608	77.9985	77.9959
950	85.0103	84.9943	84.8998	84.7242	84.8895	84.6986	84.9377	84.935
1000	92.089	92.0723	91.977	91.8027	91.9662	91.7762	92.0166	92.0138

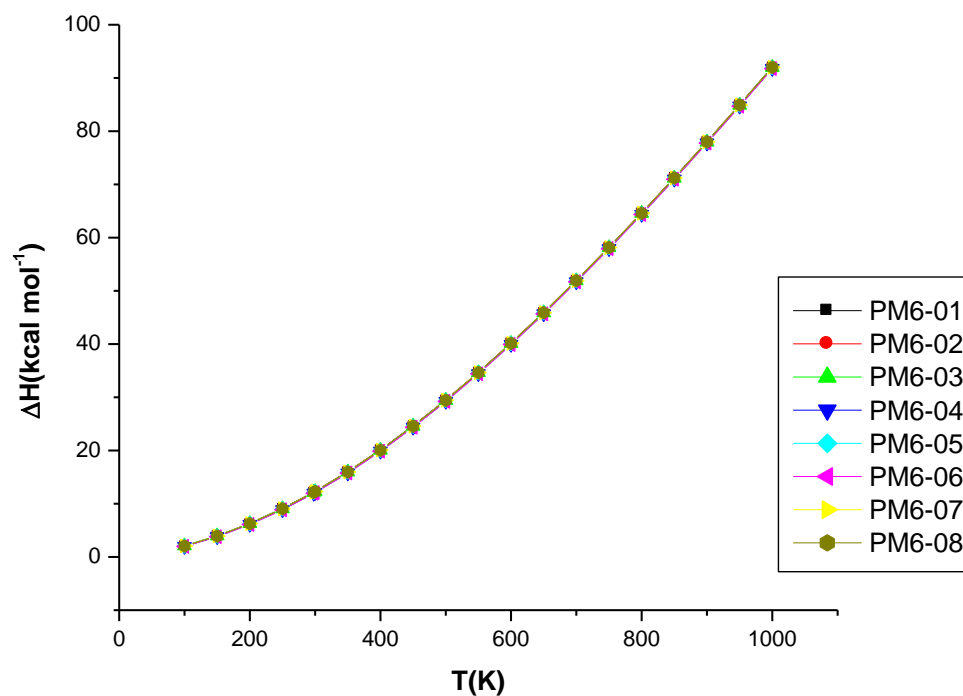


Fig. 7. Functional dependencies ΔH graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM6-M12

Table 8.

M12 Polinomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of ΔH for distinct conformers with geometry optimized by the PM6 hamiltonian

Conformerul	a_0	a_1	$a_2 \cdot 10^4$	$a_3 \cdot 10^8$	r^2	SD	$F \cdot 10^{-6}$
PM6-01	0.0994	0.0089	1.1674	-3.3683	1.0000	0.0297	5.9913
PM6-02	0.0916	0.0089	1.1668	-3.3650	1.0000	0.0294	6.1164
PM6-03	0.1355	0.0084	1.1741	-3.3989	1.0000	0.0300	5.8636
PM6-04	0.0880	0.0077	1.1846	-3.4492	1.0000	0.0303	5.7705
PM6-05	0.1208	0.0084	1.1733	-3.3956	1.0000	0.0298	5.9761
PM6-06	0.0801	0.0077	1.1841	-3.4468	1.0000	0.0300	5.8717
PM6-07	0.1077	0.0086	1.1715	-3.3861	1.0000	0.0297	5.9981
PM6-08	0.0886	0.0086	1.1707	-3.3833	1.0000	0.0294	6.1176
Mean	0.1015	0.0084	1.1741	-3.3992	1.0000	0.0298	5.9632
SD	0.0188	0.0005	0.0068	0.0324	0.0000	0.0003	0.1224

$$\Delta H(T) = \mathbf{0.1015}(\pm 0.0188) + \mathbf{0.0084}(\pm 0.0005)T + \mathbf{1.1741}(\pm 0.0069) \cdot 10^{-4}T^2 - \mathbf{3.3992}(\pm 0.0324) \cdot 10^{-8}T^3$$

$$T \in [100K, 1000K] \text{ (SD} = \mathbf{0.0298} \pm 0.0003; \mathbf{5.9632}(\pm 0.1224) \cdot 10^6$$

$$\Delta a_0 = 0.0554 \text{ kcal} \cdot \text{mol}^{-1}$$

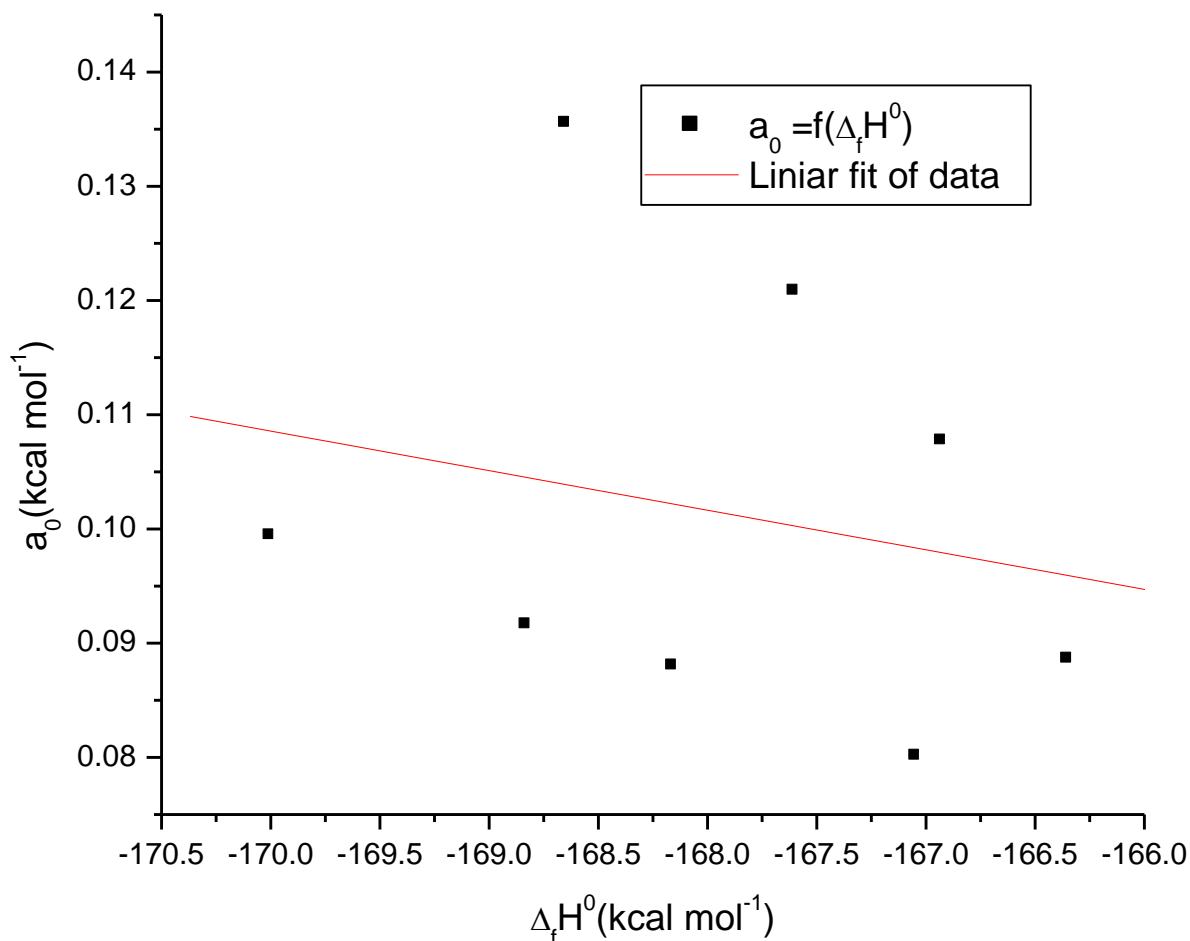


Fig. 8a. $a_0(\text{PM6}) = -0.4804 - 0.0035\Delta_f H^0(\text{PM6})$ ($r^2 = 0.0488$; SD = 0.0198; F = 0.3076)

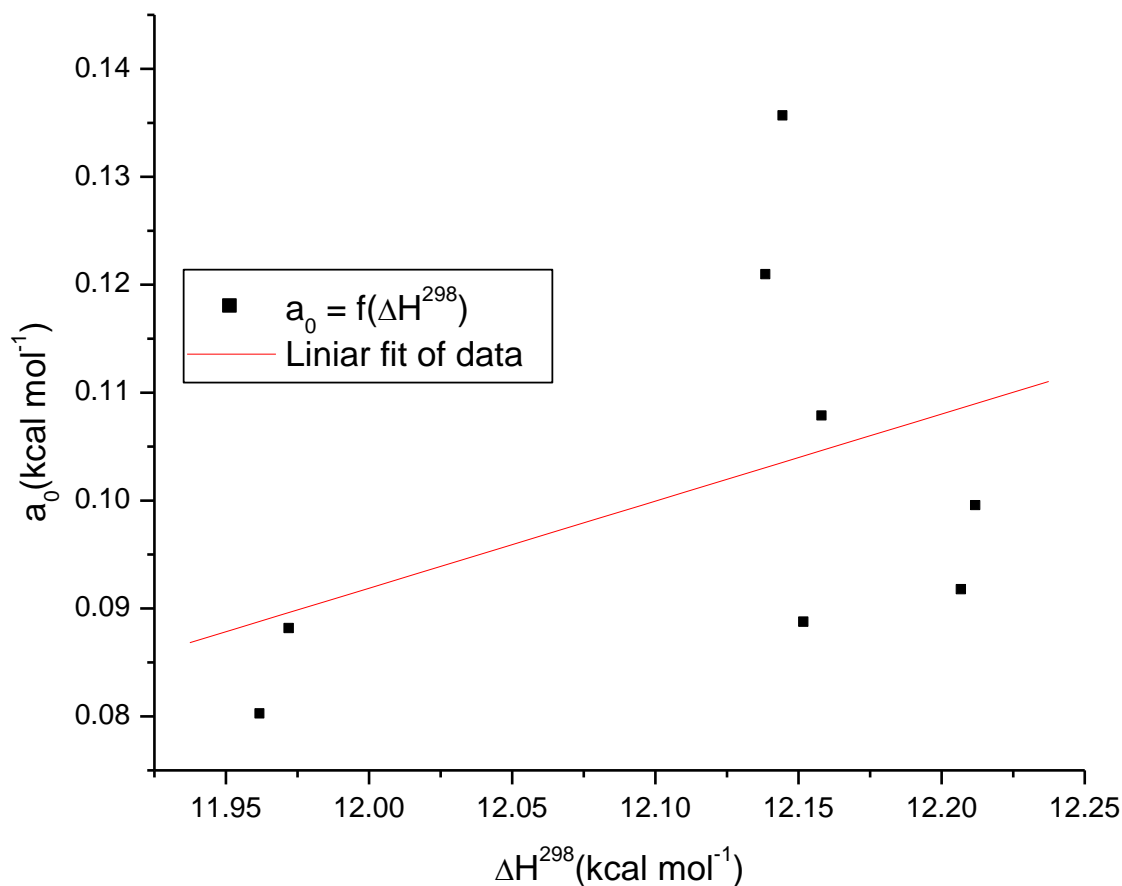


Fig. 8b. $a_0(\text{PM6}) = -0.8763 + 0.0807\Delta H^{298}(\text{PM6})$ ($r^2 = 0.0366$; SD = 0.0185; F = 1.2660)

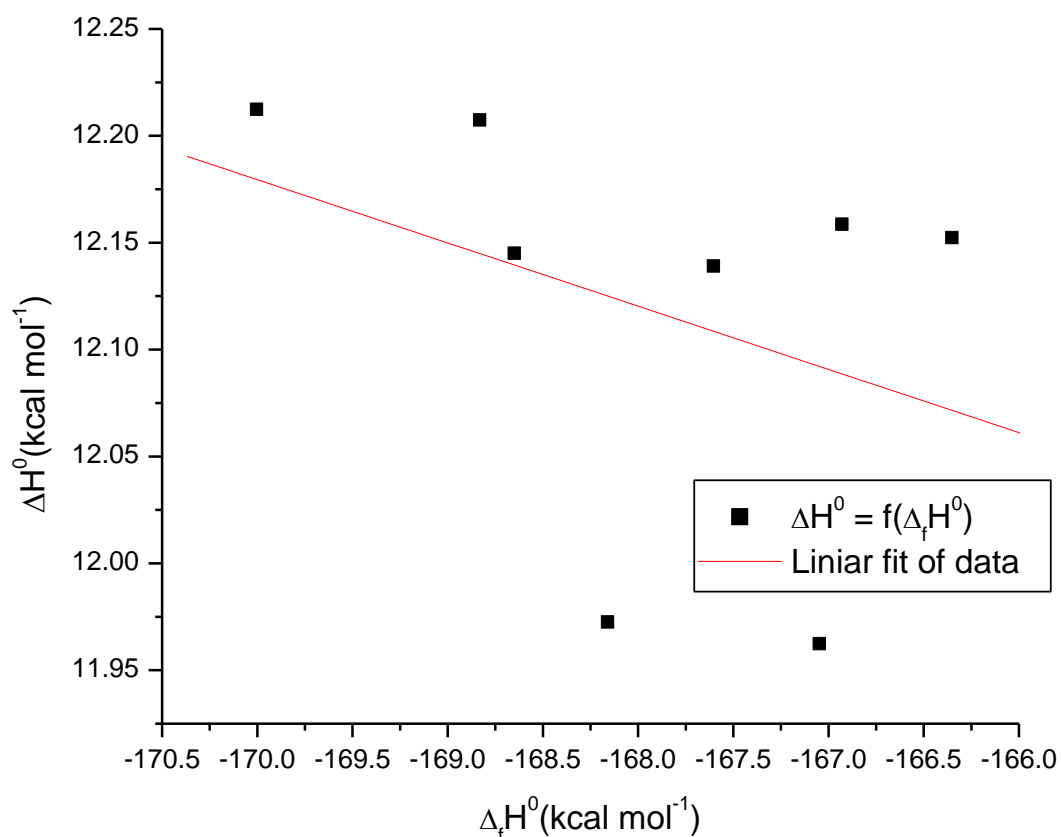


Fig. 8c. $\Delta H^0(\text{PM6}) = 7.1504 - 0.0296\Delta_f H^0(\text{PM6})$ ($r^2 = 0.1329$; SD = 0.0979; F = 0.9192)

Table 9.
 $\Delta S(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ computed by PM6-M12

Conf	PM6-01	PM6-02	PM6-03	PM6-04	PM6-05	PM6-06	PM6-07	PM6-08
T(K)								
100	90.9886	90.6704	92.0463	88.5960	91.4626	88.2415	90.9388	90.1436
150	106.1143	105.7881	107.0074	103.2906	106.4237	102.9195	105.9529	105.1622
200	119.5528	119.2259	120.3387	116.5017	119.7597	116.1250	119.3296	118.5475
250	131.9765	131.6518	132.7011	128.8032	132.1282	128.4255	131.7182	130.9455
298	143.3027	142.9794	143.9931	140.0643	143.4247	139.6858	143.0246	142.2591
300	143.7648	143.4415	144.4541	140.5244	143.8859	140.1459	143.4861	142.7209
350	155.1036	154.7802	155.7712	151.8250	155.2054	151.4447	154.8123	154.0519
400	166.0652	165.7407	166.7183	162.7637	166.1533	162.3809	165.7655	165.0081
450	176.6709	176.3446	177.3133	173.3549	176.7482	172.9693	176.3653	175.6094
500	186.9254	186.5970	187.5595	183.5997	186.9937	183.2112	186.6153	185.8602
550	196.8317	196.5012	197.4591	193.4993	196.8924	193.1080	196.5181	195.7634
600	206.3955	206.0631	207.0175	203.0584	206.4498	202.6646	206.0794	205.3248
650	215.6262	215.2920	216.2436	212.2856	215.6749	211.8896	215.3081	214.5536
700	224.5352	224.1995	225.1488	221.1921	224.5792	220.7941	224.2158	223.4612
750	233.1357	232.7986	233.7460	229.7908	233.1756	229.3910	232.8153	232.0606
800	241.4413	241.1030	242.0488	238.0951	241.4777	237.6938	241.1204	240.3656
850	249.4660	249.1266	250.0711	246.1188	249.4993	245.7162	249.1447	248.3898
900	257.2232	256.8828	257.8263	253.8754	257.2538	253.4716	256.9018	256.1467
950	264.7261	264.3849	265.3274	261.3779	264.7544	260.9730	264.4048	263.6496
1000	271.9874	271.6455	272.5872	268.6389	272.0136	268.2331	271.6662	270.9109

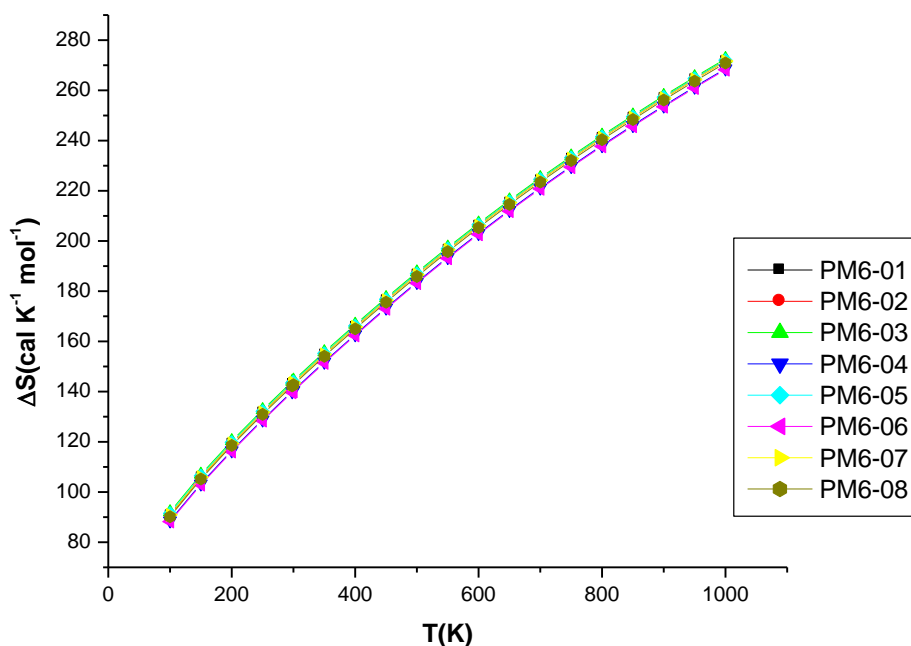


Fig. 9. Functional dependencies ΔS graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM6-M12

Table 10.

M12 Polinomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of ΔS for distinct conformers with geometry optimized by the PM6 hamiltonian

Conformer	a_0	a_1	$a_2 \cdot 10^4$	$a_3 \cdot 10^8$	r^2	SD	$F \cdot 10^{-5}$
PM6-01	62.3315	0.3087	-1.3694	3.8182	0.9999	0.3724	1.40569
PM6-02	62.0071	0.3087	-1.3703	3.8230	0.9999	0.3707	1.41823
PM6-03	63.6086	0.3056	-1.3216	3.5832	0.9999	0.3498	1.58779
PM6-04	60.4094	0.3015	-1.2552	3.2479	1.0000	0.3104	2.01029
PM6-05	63.0057	0.3058	-1.3246	3.5971	0.9999	0.3487	1.59753
PM6-06	60.0599	0.3014	-1.2539	3.2424	1.0000	0.3077	2.04470
PM6-07	60.0599	0.3014	-1.2539	3.2424	1.0000	0.3077	2.04470
PM6-08	60.0599	0.3014	-1.2539	3.2424	1.0000	0.3077	2.04470
Mean	61.4428	0.3043	-1.3004	3.4746	0.9999	0.3344	1.7692
SD	1.4661	0.0033	0.0524	0.2617	0.0001	0.0291	1.4057

$$\Delta S(T) = 61.4428(\pm 1.4661) + 0.3043(\pm 0.0033)T - 1.3004(\pm 0.0524) \cdot 10^{-4}T^2 + 3.4746(\pm 0.2617) \cdot 10^{-8}T^3$$

$$T \in [100K, 1000K] \text{ (SD} = 0.3344 \pm 0.0291; 1.7692(\pm 1.4057) \cdot 10^5$$

$$\Delta a_0 = 3.5487 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

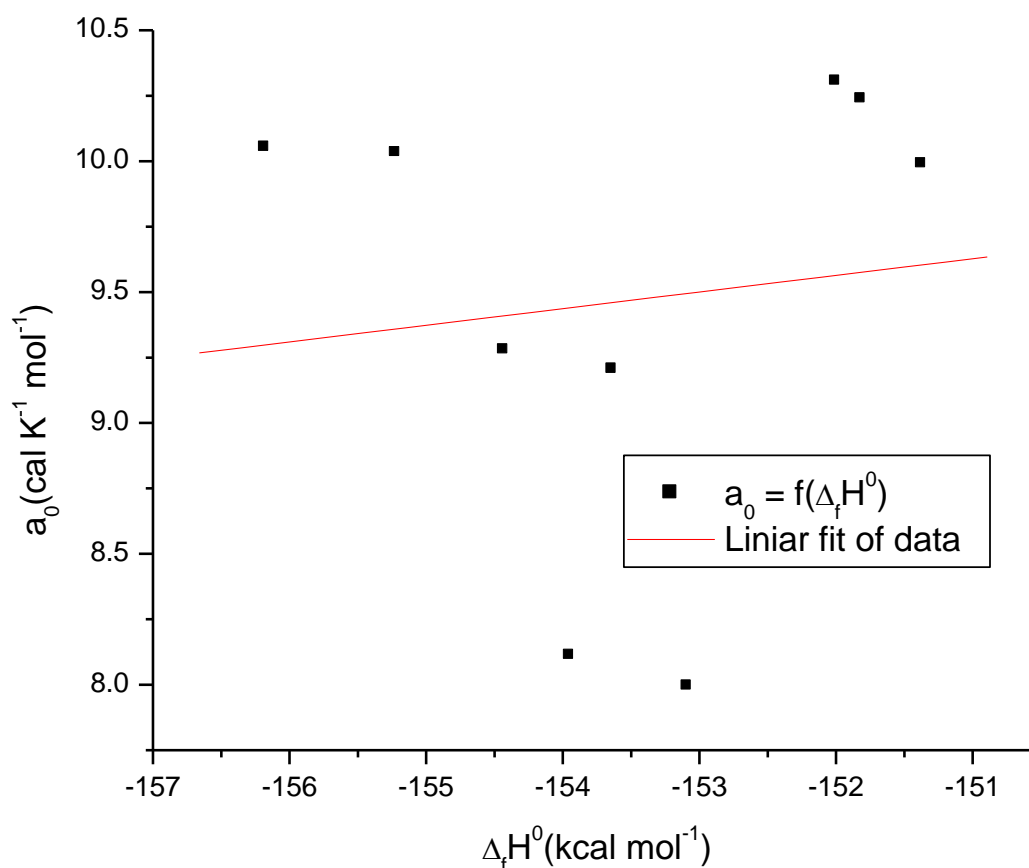


Fig. 10a. $a_0(\text{PM6}) = 19.23047 + 3.8974\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0134$; SD = 0.9456; F = 0.0950)

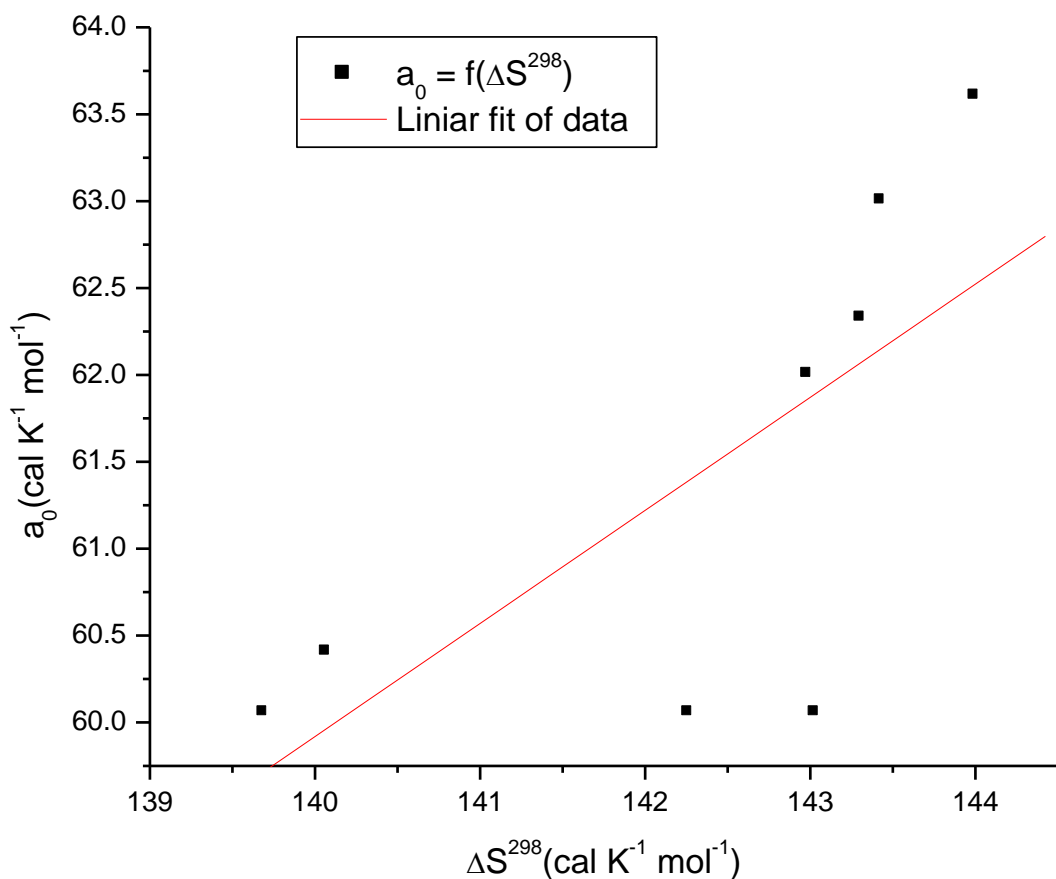


Fig. 10b. $a_0(\text{PM6}) = -31.2051 + 0.6509\Delta S^0(\text{PM6})$ ($r^2 = 0.4228$; $\text{SD} = 1.1139$; $F = 6.1265$)

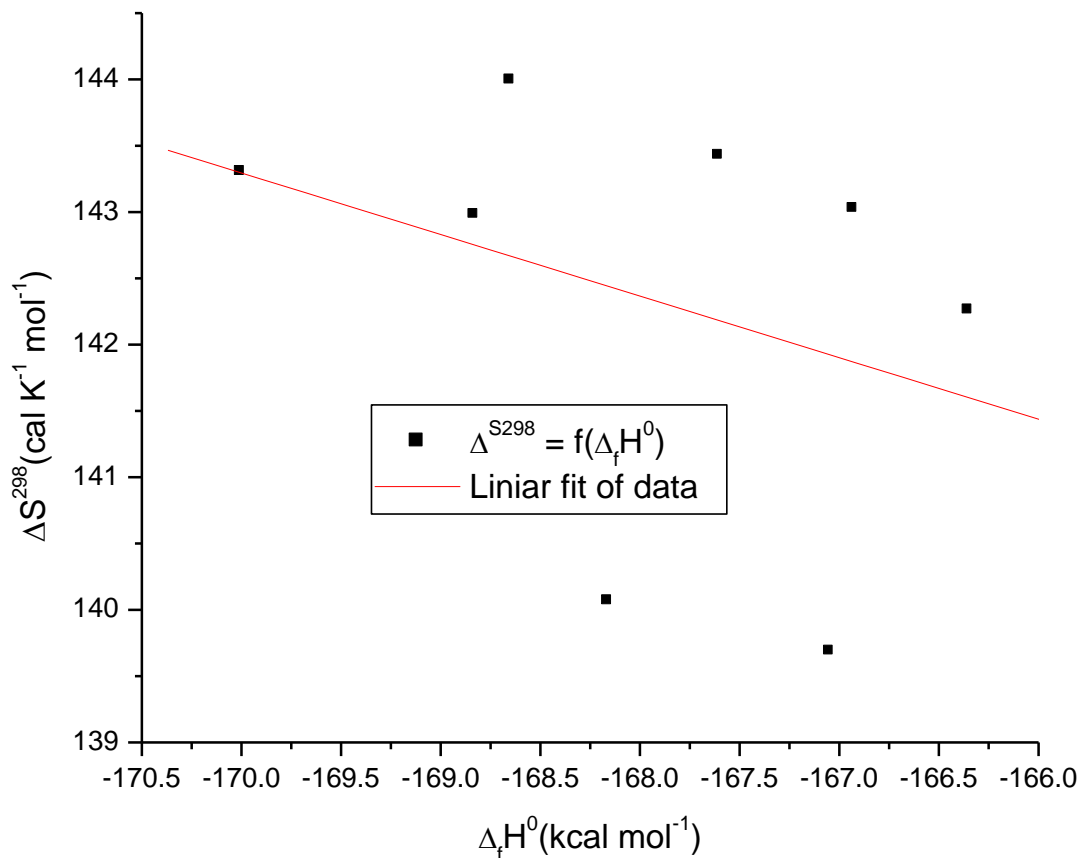


Fig. 10c. $\Delta S^0(\text{PM6}) = 64.3877 - 0.4642\Delta_f H^0(\text{PM6})$ ($r^2 = 0.1208$; $\text{SD} = 1.6215$; $F = 0.8242$)

Table 11.
 $C_p(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ computed by PM6-M12

Conf	PM6-01	PM6-02	PM6-03	PM6-04	PM6-05	PM6-06	PM6-07	PM6-08
T(K)								
100	32.6565	32.6350	32.2803	31.4679	32.2781	31.4235	32.3531	32.3624
150	42.4091	42.3972	41.9997	41.4910	42.0072	41.4601	42.1661	42.1853
200	51.3915	51.3980	51.0688	50.7366	51.0936	50.7276	51.2081	51.2469
250	60.3080	60.3186	60.0803	59.8640	60.1083	59.8615	60.1766	60.2201
298	68.9110	68.9155	68.7472	68.6087	68.7683	68.6017	68.8157	68.8528
300	69.2673	69.2714	69.1055	68.9697	69.1263	68.9624	69.1732	69.2099
350	78.0079	78.0028	77.8860	77.8048	77.8967	77.7896	77.9374	77.9638
400	86.2581	86.2453	86.1598	86.1147	86.1617	86.0927	86.2021	86.2192
450	93.8676	93.8496	93.7839	93.7626	93.7796	93.7362	93.8213	93.8315
500	100.7968	100.7761	100.7232	100.7175	100.7149	100.6889	100.7579	100.7635
550	107.0715	107.0496	107.0054	107.0101	106.9949	106.9811	107.0390	107.0416
600	112.7456	112.7237	112.6859	112.6975	112.6742	112.6690	112.7190	112.7198
650	117.8806	117.8592	117.8263	117.8427	117.8141	117.8153	117.8595	117.8591
700	122.5350	122.5145	122.4855	122.5052	122.4734	122.4792	122.5190	122.5179
750	126.7614	126.7420	126.7163	126.7382	126.7044	126.7137	126.750	126.7485
800	130.6056	130.5873	130.5646	130.5879	130.5530	130.5649	130.5985	130.5966
850	134.1078	134.0905	134.0703	134.0945	134.0592	134.0729	134.1043	134.1022
900	137.3027	137.2864	137.2684	137.2930	137.2578	137.2729	137.3023	137.3000
950	140.2210	140.2057	140.1896	140.2144	140.1795	140.1955	140.2232	140.2209
1000	142.8899	142.8755	142.8612	142.8858	142.8515	142.8681	142.894	142.8919

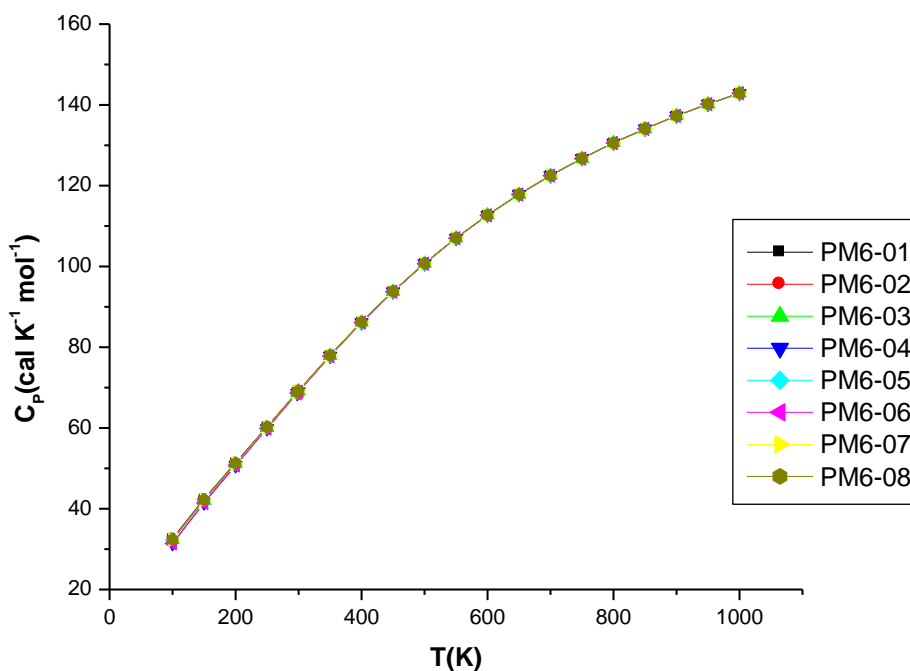


Fig. 11. Functional dependencies C_p graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM6-M12

Table 12.

M12 Polinomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of $C_p(T)$ for distinct conformers with geometry optimized by the PM6 hamiltonian

Conformerul	a_0	a_1	$a_2 \cdot 10^5$	$a_3 \cdot 10^{10}$	r^2	SD	F
PM6-01	10.1069	0.2280	-9.6071	2.4776	0.9997	0.5513	25245.5
PM6-02	10.0794	0.2282	-9.6602	5.8803	0.9998	0.5439	25924.1
PM6-03	9.4783	0.2302	-9.9012	15.2665	0.9997	0.5529	25248.6
PM6-04	8.2404	0.2361	-10.7788	57.3808	0.9998	0.5222	28609.1
PM6-05	9.4710	0.2304	-9.9582	18.9251	0.9998	0.5455	25924.0
PM6-06	8.1824	0.2364	-10.8445	61.3696	0.9998	0.5144	29486.9
PM6-07	9.6467	0.2298	-9.8677	14.6983	0.9998	0.5441	26032.3
PM6-08	9.6455	0.2301	-9.9366	18.9583	0.9998	0.5364	26768.9
Mean	9.3563	0.2312	-10.0693	24.3696	0.9998	0.5388	26654.93
SD	0.7470	0.0033	0.4757	22.4091	0.0000	0.0138	1570.81

$$C_p(T) = 9.3563(\pm 0.7470) + 0.2312(\pm 0.0033)T - 10.0693(\pm 0.4757) \cdot 10^{-5}T^2 + 24.3696(\pm 22.4091) \cdot 10^{-10}T^3$$

$$T \in [100K, 1000K] \text{ (SD} = 0.5388 \pm 0.0138; 26654.93(\pm 1570.81))$$

$$\Delta a_0 = 1.9245 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

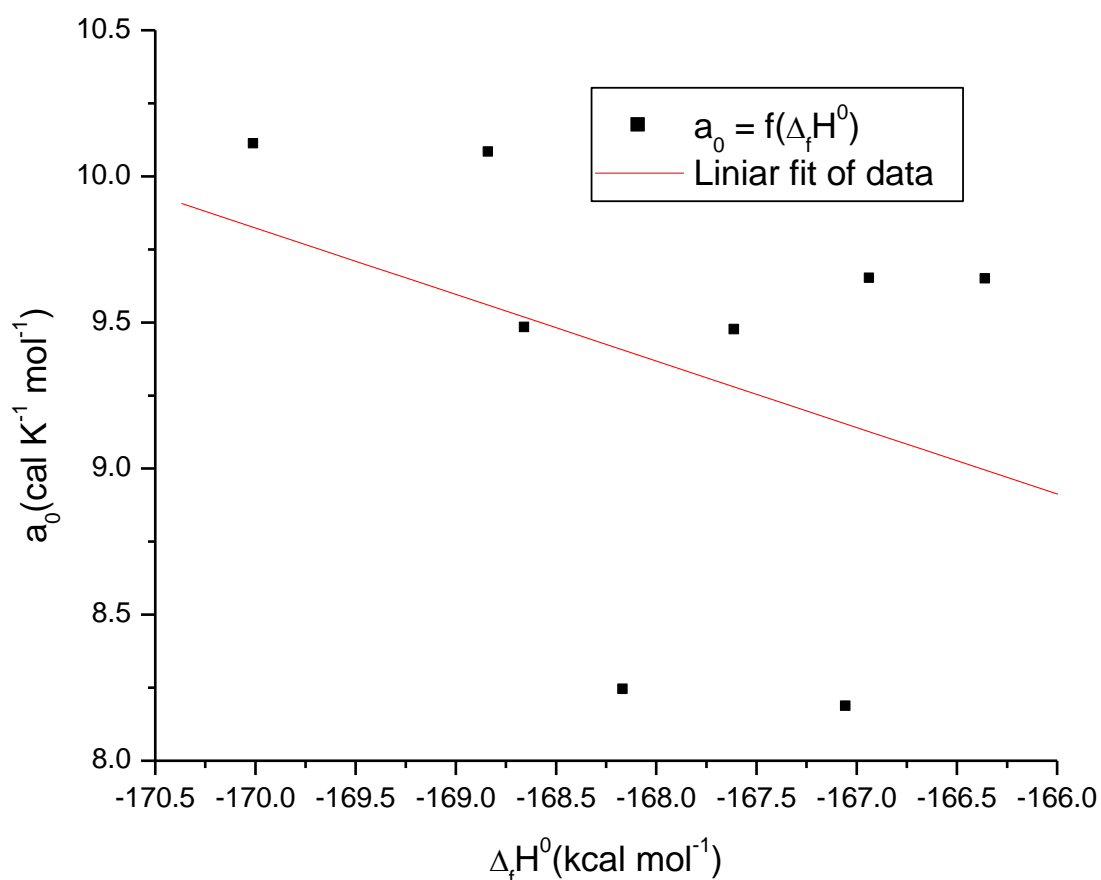


Fig. 12a. $a_0(\text{PM6}) = -28.8758 - 0.2276\Delta_f H^0(\text{PM6})$ ($r^2 = 0.1334$; SD = 0.7510; F = 0.9242)

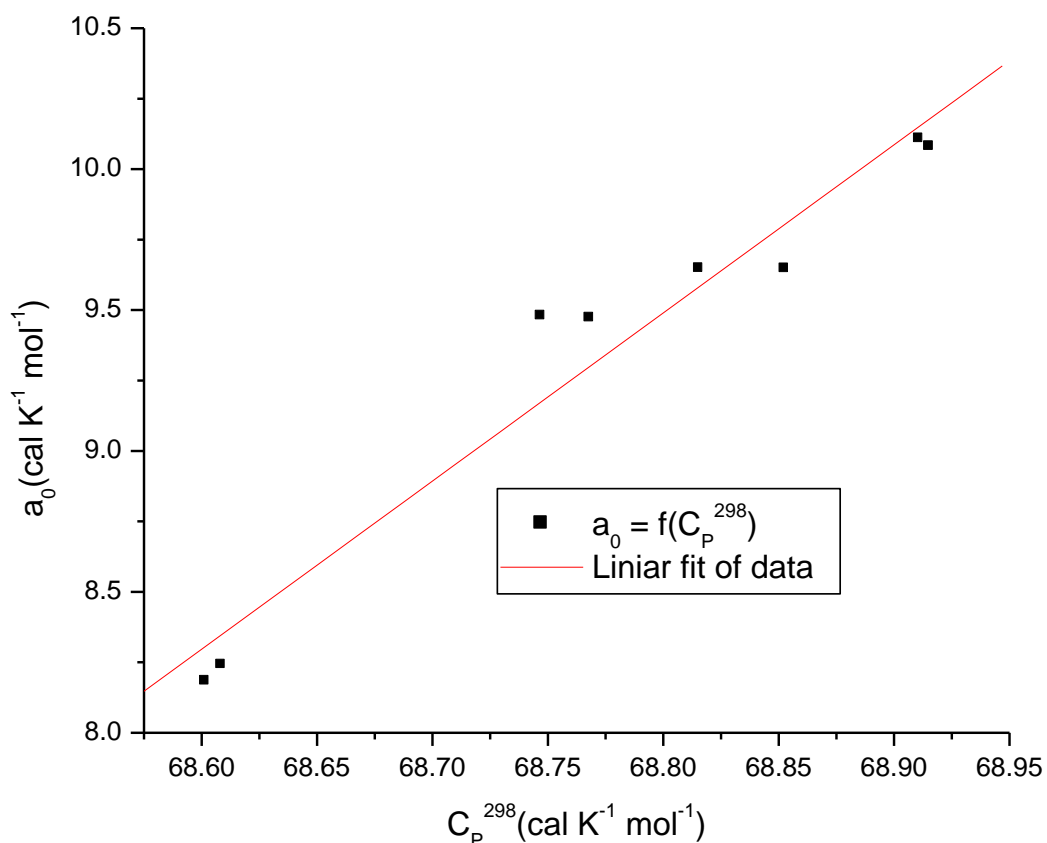


Fig. 12b. $a_0(\text{PM6}) = -400.9790 + 5.9661C_p^{298}(\text{PM6})$ ($r^2 = 0.9434$; $\text{SD} = 0.1777$; $F = 117.6066$)

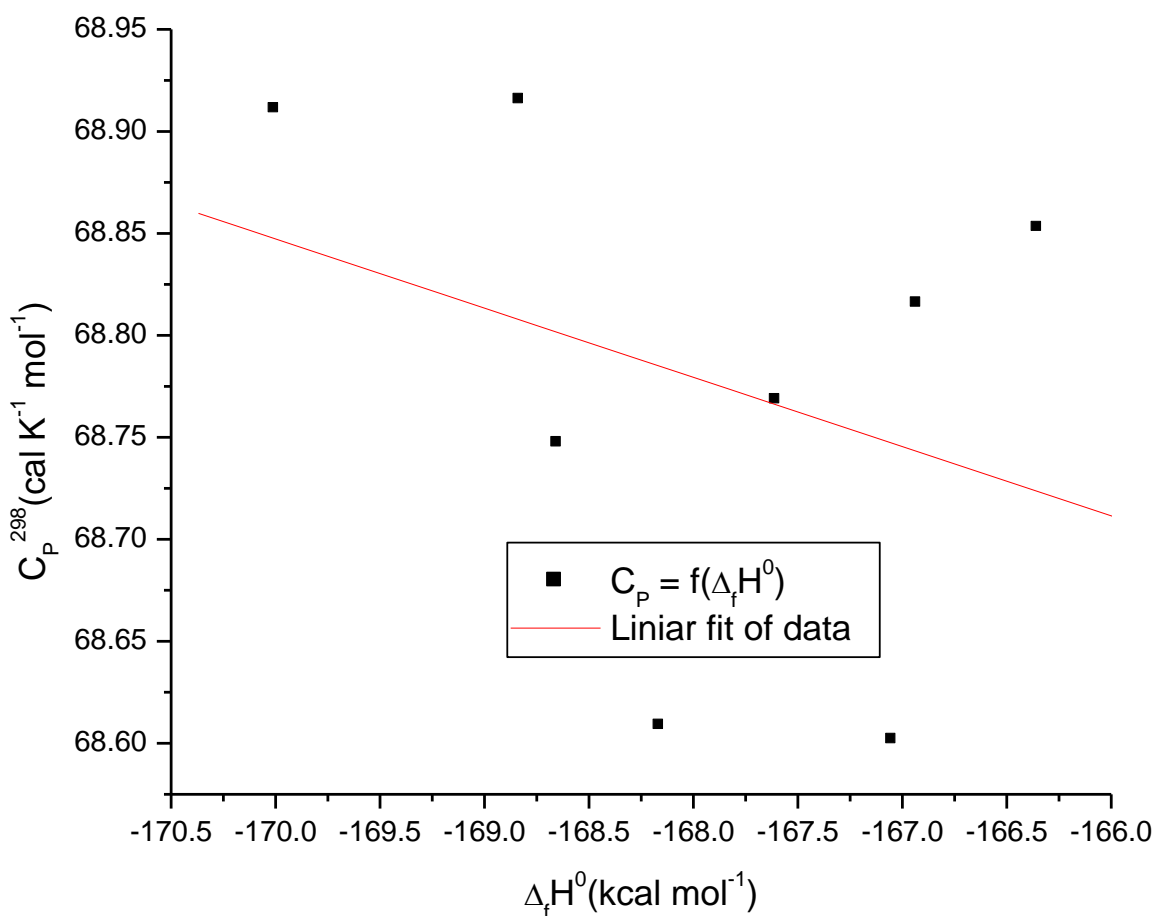


Fig. 12c. $C_p(\text{PM6}) = 63.0768 - 0.0339\Delta_f H^0(\text{PM6})$ ($r^2 = 0.1110$; $\text{SD} = 0.1243$; $F = 0.7493$)

Table 13.
 $\Delta H(\text{kcal}\cdot\text{mol}^{-1}) = f(T)$ computed by PM7-M12

Conf	PM7-01	PM7-02	PM7-03	PM7-04	PM7-05	PM7-06	PM7-07	PM7-08	PM7-09
T(K)									
100	2.0646	2.0643	2.0341	1.9435	2.0271	1.9377	2.0563	2.0875	2.0523
150	3.9253	3.924	3.8708	3.75	3.8617	3.7401	3.9312	3.9576	3.9152
200	6.2546	6.2529	6.1796	6.04	6.1694	6.0272	6.2758	6.2971	6.2505
250	9.0283	9.0267	8.9378	8.7865	8.9276	8.7719	9.0633	9.0805	9.0316
298	12.1056	12.104	12.0043	11.8463	11.9941	11.8301	12.1528	12.1662	12.1157
300	12.2426	12.2409	12.1409	11.9827	12.1307	11.9665	12.2903	12.3035	12.253
350	15.8918	15.8896	15.7817	15.6196	15.7712	15.6016	15.9511	15.9603	15.9082
400	19.9587	19.9555	19.842	19.6779	19.8307	19.658	20.0288	20.0337	19.9797
450	24.4167	24.4122	24.2945	24.1297	24.2821	24.1076	24.4967	24.4971	24.4411
500	29.2348	29.2288	29.1078	28.943	29.0941	28.9187	29.3238	29.3196	29.2614
550	34.3814	34.3738	34.2502	34.0858	34.2351	34.0593	34.4783	34.4696	34.4093
600	39.8264	39.8172	39.6914	39.5278	39.6749	39.4992	39.9304	39.9173	39.855
650	45.5424	45.5316	45.4039	45.2413	45.3861	45.2106	45.6526	45.6354	45.5712
700	51.5045	51.4922	51.3629	51.2014	51.3438	51.1688	51.6201	51.5991	51.5332
750	57.6904	57.6767	57.5461	57.3857	57.5257	57.3514	57.8108	57.7861	57.7187
800	64.0801	64.0651	63.9333	63.7741	63.9117	63.7382	64.2046	64.1767	64.1079
850	70.6556	70.6394	70.5066	70.3487	70.4839	70.3112	70.7837	70.7528	70.6828
900	77.4007	77.3834	77.2497	77.093	77.226	77.0542	77.532	77.4983	77.4272
950	84.3008	84.2824	84.148	83.9925	84.1234	83.9524	84.4347	84.3987	84.3265
1000	91.3426	91.3233	91.1882	91.034	91.1627	90.9927	91.4789	91.4406	91.3676

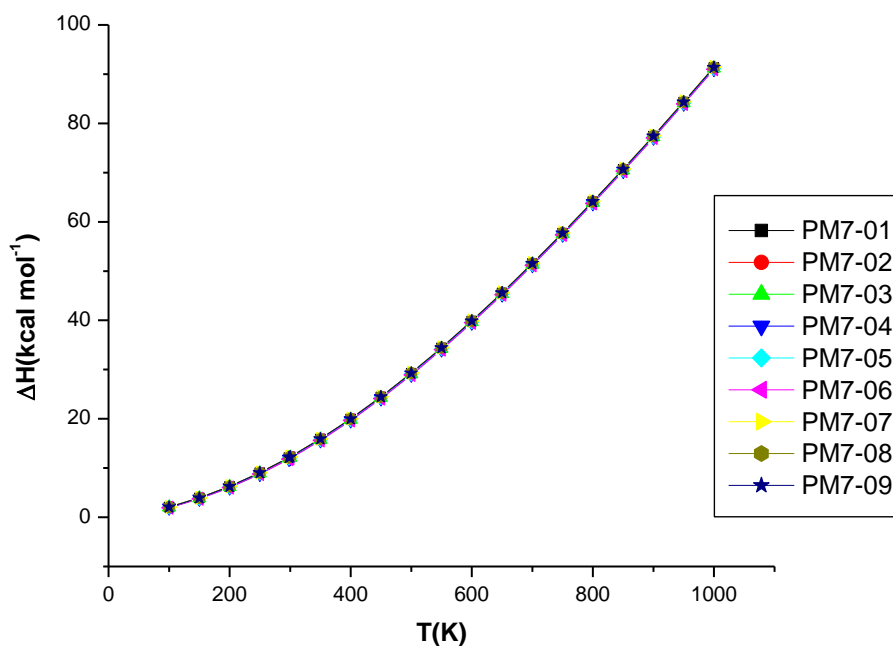


Fig. 13. Functional dependencies ΔH graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM7-M12

Table 14.

MOPAC12 Polinomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of ΔH for distinct conformers with geometry optimized by the PM7 hamiltonian

Conformerul	a_0	a_1	$a_2 \cdot 10^4$	$a_3 \cdot 10^8$	r^2	SD	$F \cdot 10^{-6}$
PM7-01	0.0542	0.0092	1.1453	-3.2504	1.0000	0.0254	8.0723
PM7-02	0.0513	0.0093	1.1444	-3.2459	1.0000	0.0251	8.2662
PM7-03	0.0706	0.0086	1.1527	-3.2838	1.0000	0.0256	7.9101
PM7-04	0.0240	0.0080	1.1625	-3.3313	1.0000	0.0230	7.7195
PM7-05	0.0621	0.0087	1.1522	-3.2816	1.0000	0.0254	8.0940
PM7-06	0.0216	0.0080	1.1625	-3.3307	1.0000	0.0258	7.8270
PM7-07	0.0097	0.0096	1.1428	-3.2453	1.0000	0.0254	8.0994
PM7-08	0.0480	0.0095	1.1424	-3.2411	1.0000	.0252	8.2553
PM7-09	0.0183	0.0094	1.1431	-3.2439	1.0000	0.0247	8.5585
Mean	0.0400	0.0089	1.1498	-3.2727	1.0000	0.0251	8.0891
SD	0.0218	0.0006	0.0082	0.0367	0.0000	0.0008	0.2542

$$\Delta H(T) = 0.0400(\pm 0.0218) + 0.0089(\pm 0.0006)T + 1.1498(\pm 0.0082) \cdot 10^{-4}T^2 - 3.2727(\pm 0.0367) \cdot 10^{-8}T^3$$

$$T \in [100K, 1000K] \quad (SD = 0.0251 \pm 0.0008; 8.0891(\pm 0.2542) \cdot 10^6)$$

$$\Delta a_0 = 0.0609 \text{ kcal} \cdot \text{mol}^{-1}$$

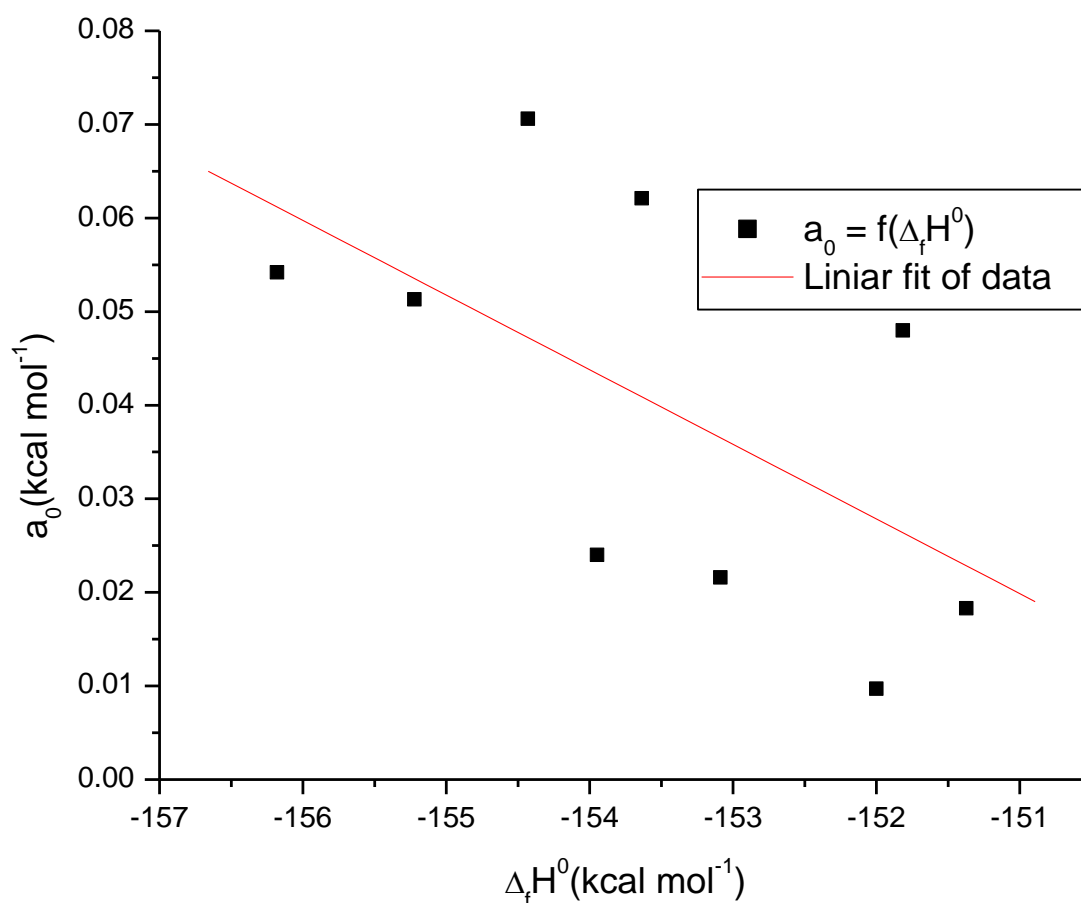


Fig. 14a. $a_0(\text{PM7}) = -1.1843 - 0.0080\Delta_f H^0(\text{PM7})$ ($r^2 = 0.3514$; $SD = 0.0188$; $F = 3.7932$)

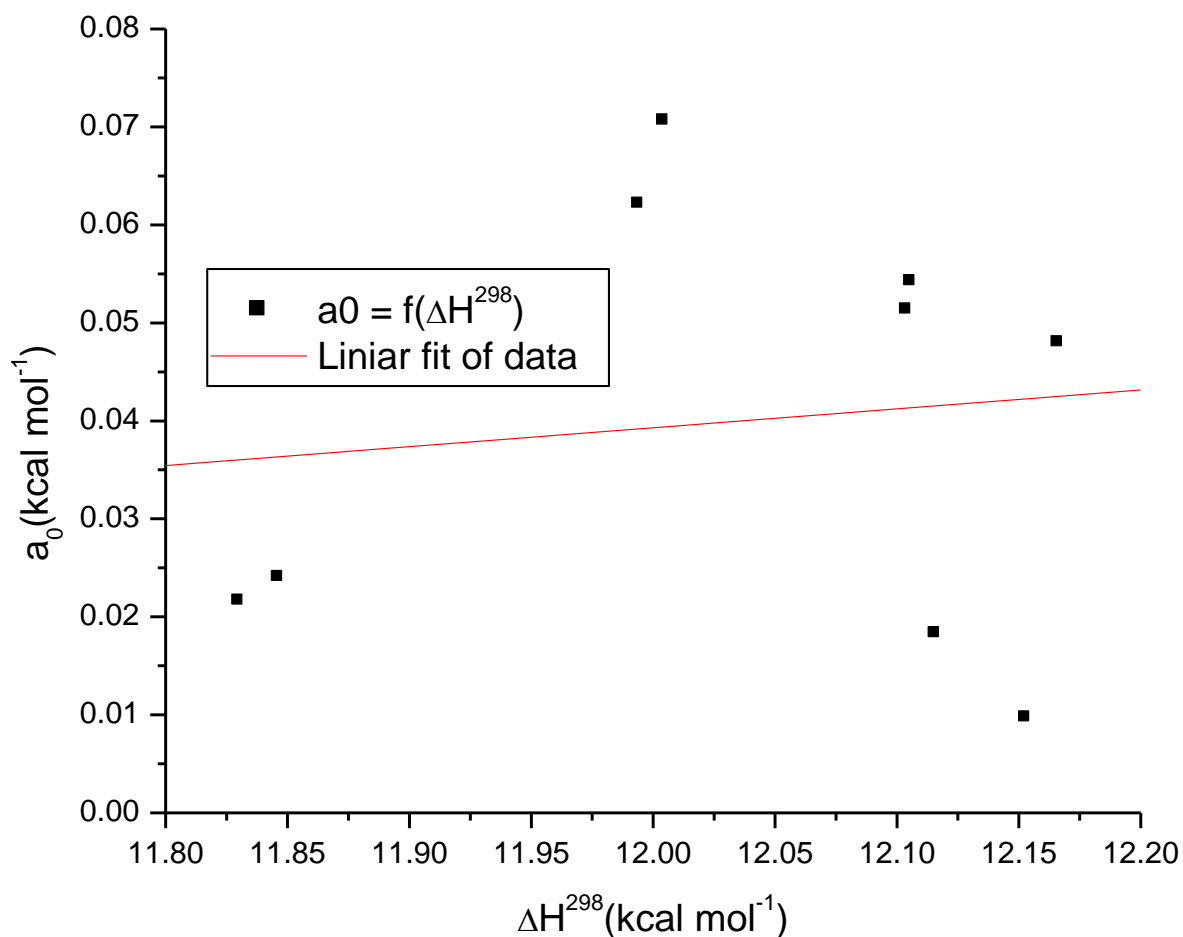


Fig. 14b. $a_0(\text{PM7}) = -0.1919 + 0.0193\Delta H^0(\text{PM7})$ ($r^2 = 0.0125$; $\text{SD} = 0.0232$; $F = 0.0883$)

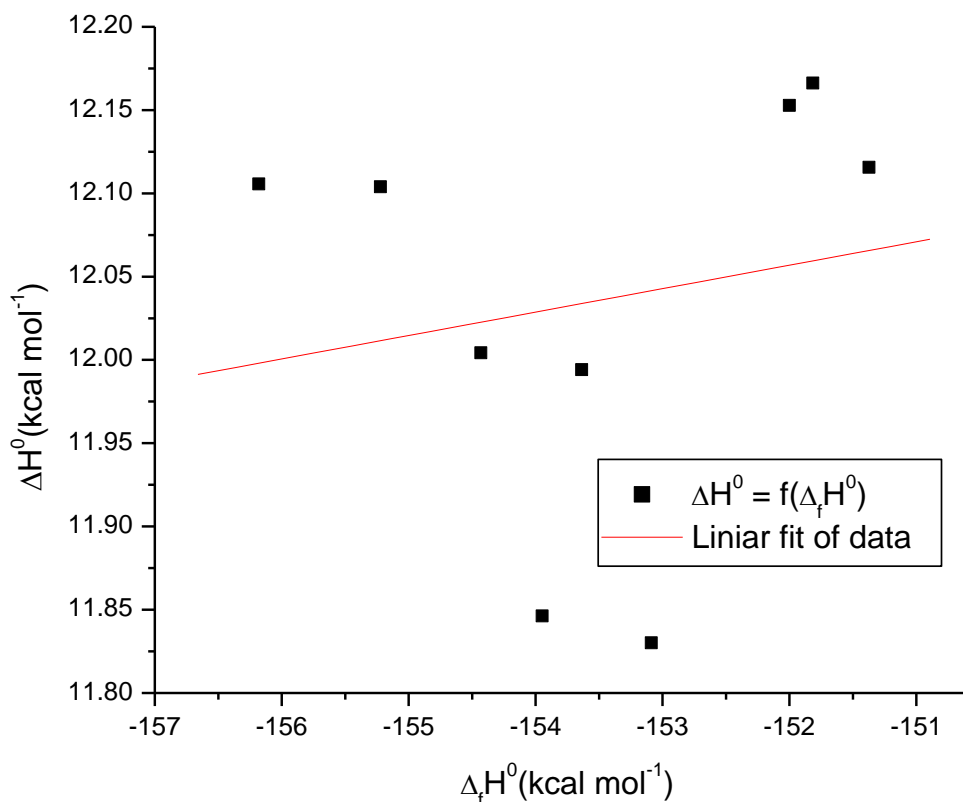


Fig. 14c. $a_0(\text{PM7}) = 14.1961 + 0.0141\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0326$; $\text{SD} = 0.1328$; $F = 0.2360$)

Table 15.
 $\Delta S(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ computed by PM7-MOPAC12

Conf	PM7-01	PM7-02	PM7-03	PM7-04	PM7-05	PM7-06	PM7-07	PM7-08	PM7-09
T(K)									
100	90.4030	90.3704	90.7402	87.3534	90.5116	87.2020	89.6023	91.1509	89.7597
150	105.3573	105.3161	105.4996	101.8646	105.2527	101.6795	104.6709	106.1811	104.7305
200	118.6973	118.6539	118.7204	114.9759	118.4684	114.7744	118.0988	119.5797	118.1047
250	131.0395	130.9965	130.9931	127.1959	130.7407	126.9861	130.5029	131.9648	130.4797
298	142.2777	142.2344	142.1916	138.3694	141.9392	138.1541	141.7856	143.2338	141.7430
300	142.7359	142.6926	142.6484	138.8256	142.3961	138.6101	142.2454	143.6931	142.2021
350	153.9693	153.9244	153.8561	150.0211	153.6026	149.8002	153.5149	154.9502	153.4542
400	164.8184	164.7709	164.6875	160.8472	164.4320	160.6211	164.3928	165.8168	164.3157
450	175.3114	175.2608	175.1674	171.3254	174.9093	171.0941	174.9091	176.3224	174.8165
500	185.4578	185.4040	185.3037	181.4617	185.0429	181.2257	185.0743	186.4780	184.9676
550	195.2635	195.2066	195.1013	191.2602	194.8379	191.0200	194.8952	196.2903	194.7759
600	204.7354	204.6758	204.5666	200.7269	204.3008	200.4830	204.3795	205.7669	204.2491
650	213.8831	213.8210	213.7088	209.8706	213.4408	209.6235	213.5371	214.9180	213.3971
700	222.7177	222.6534	222.5389	218.7023	222.2689	218.4523	222.3798	223.7549	222.2315
750	231.2517	231.1854	231.0690	227.2341	230.7973	226.9816	230.9204	232.2905	230.7650
800	239.4980	239.4301	239.3121	235.4787	239.0389	235.2242	239.1720	240.5379	239.0106
850	247.4697	247.4003	247.2811	243.4492	247.0066	243.1928	247.1480	248.5103	246.9815
900	255.1796	255.1089	254.9887	251.1582	254.7131	250.9003	254.8615	256.2207	254.6906
950	262.6402	262.5684	262.4474	258.6183	262.1707	258.3590	262.3251	263.6816	262.1505
1000	269.8636	269.7908	269.6692	265.8413	269.3916	265.5808	269.5509	270.9051	269.3731

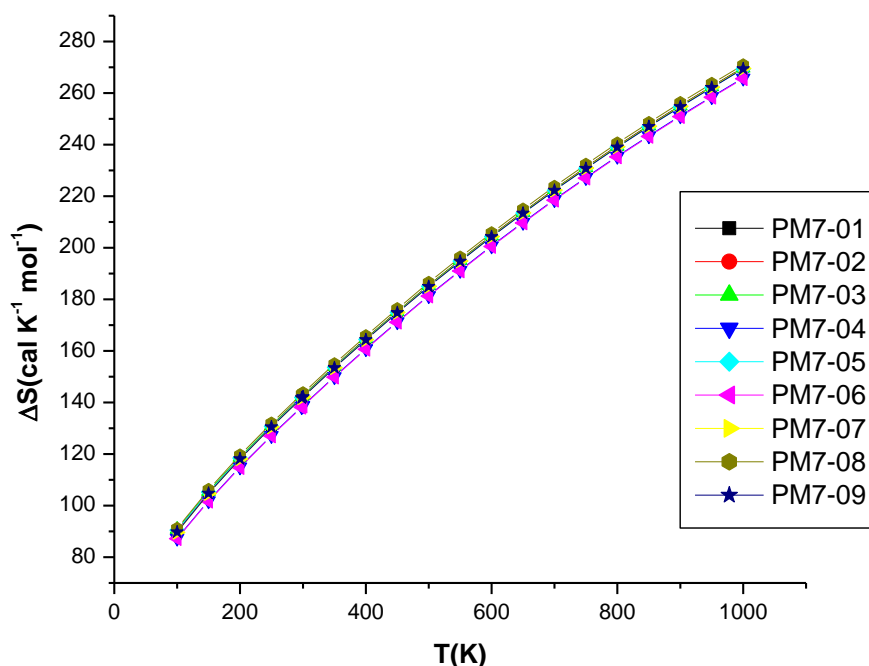


Fig. 15. Functional dependencies ΔS graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM7-MOPAC12

Table 16.

MOPAC12 Polynomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of ΔS for distinct conformers with geometry optimized by the PM7 hamiltonian

Conformerul	a_0	a_1	$a_2 \cdot 10^4$	$a_3 \cdot 10^8$	r^2	SD	$F \cdot 10^{-5}$
PM7-01	61.9202	0.3068	-1.3773	3.9233	1.0000	0.3647	1.44015
PM7-02	61.8858	0.3067	-1.3780	3.9285	1.0000	0.3633	1.45025
PM7-03	62.5066	0.3032	-1.3227	3.6564	1.0000	0.3381	1.66832
PM7-04	59.3422	0.2995	-1.2618	3.3463	1.0000	0.3002	2.11130
PM7-05	62.2810	0.3030	-1.3214	3.6505	1.0000	0.3350	1.69880
PM7-06	59.2202	0.2990	-1.2559	3.3192	1.0000	0.2957	2.17489
PM7-07	60.9149	0.3093	-1.4107	4.0722	1.0000	0.3743	1.37293
PM7-08	62.5213	0.3086	-1.4024	4.0374	1.0000	0.3704	1.39942
PM7-09	61.1723	0.3078	-1.3916	3.9847	1.0000	0.3615	1.46764
Mean	61.3072	0.3049	-1.3469	3.7687	1.0000	0.3448	1.6426
SD	1.2728	0.0039	0.0589	0.2888	0.0000	0.0298	0.3056

$$\Delta S(T) = 61.3072(\pm 1.2728) + 0.3049(\pm 0.0039)T - 1.3469(\pm 0.0589) \cdot 10^{-4}T^2 + 3.7687(\pm 0.2888) \cdot 10^{-8}T^3$$

$$T \in [100K, 1000K] \text{ (SD} = 0.3448 \pm 0.0298; 1.6426(\pm 0.3056) \cdot 10^5$$

$$\Delta a_0 = 3.3011 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

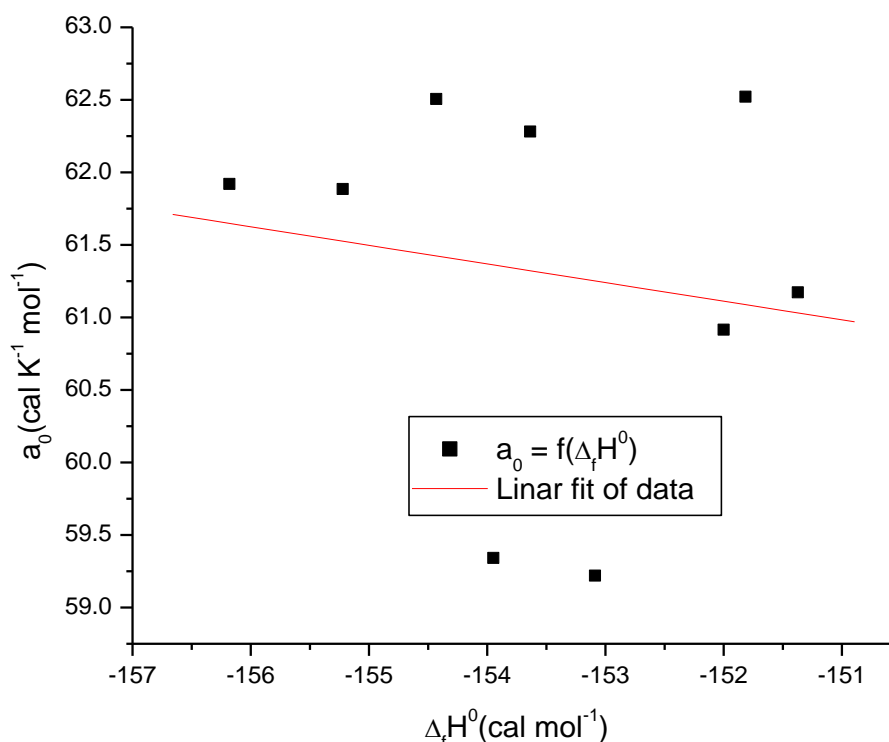


Fig. 16a. $a_0(\text{PM7}) = 41.5950 - 0.1284\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0267$; SD = 1.3424; F = 0.1922)

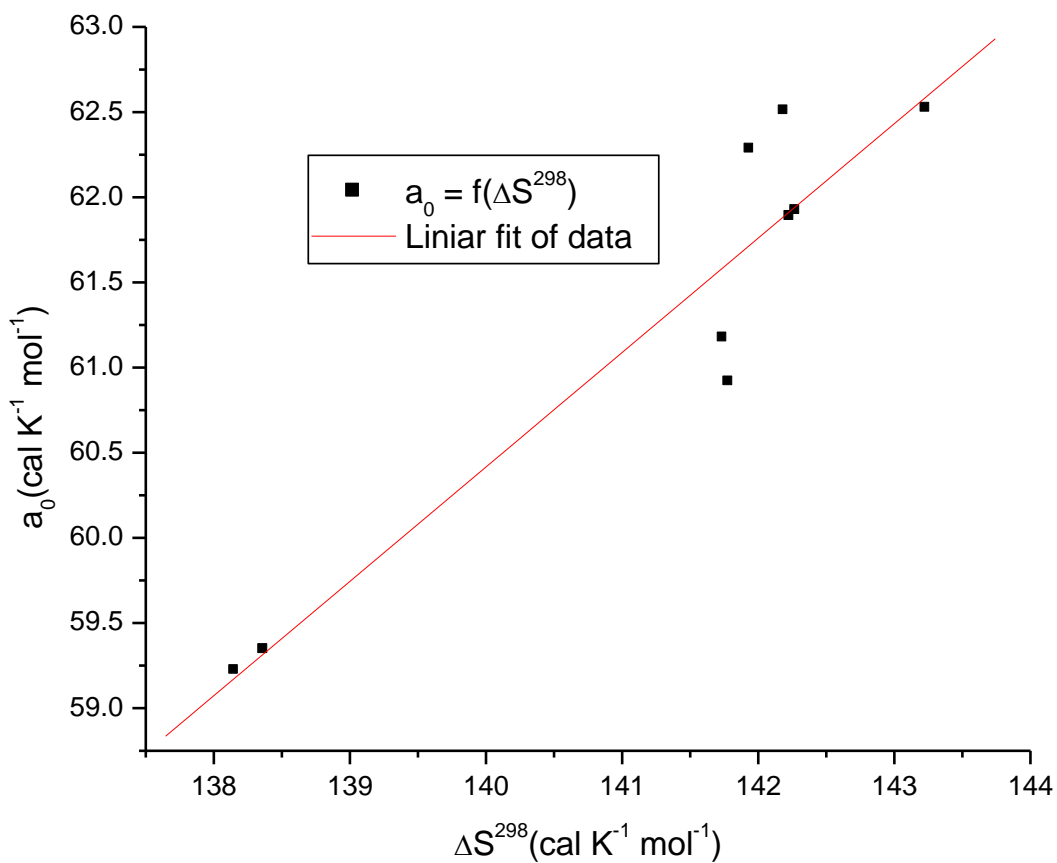


Fig. 16b. $a_0(\text{PM7}) = -33.6318 + 0.6718\Delta S^0(\text{PM7})$ ($r^2 = 0.8792$; SD = 0.4424; F = 59.2281)

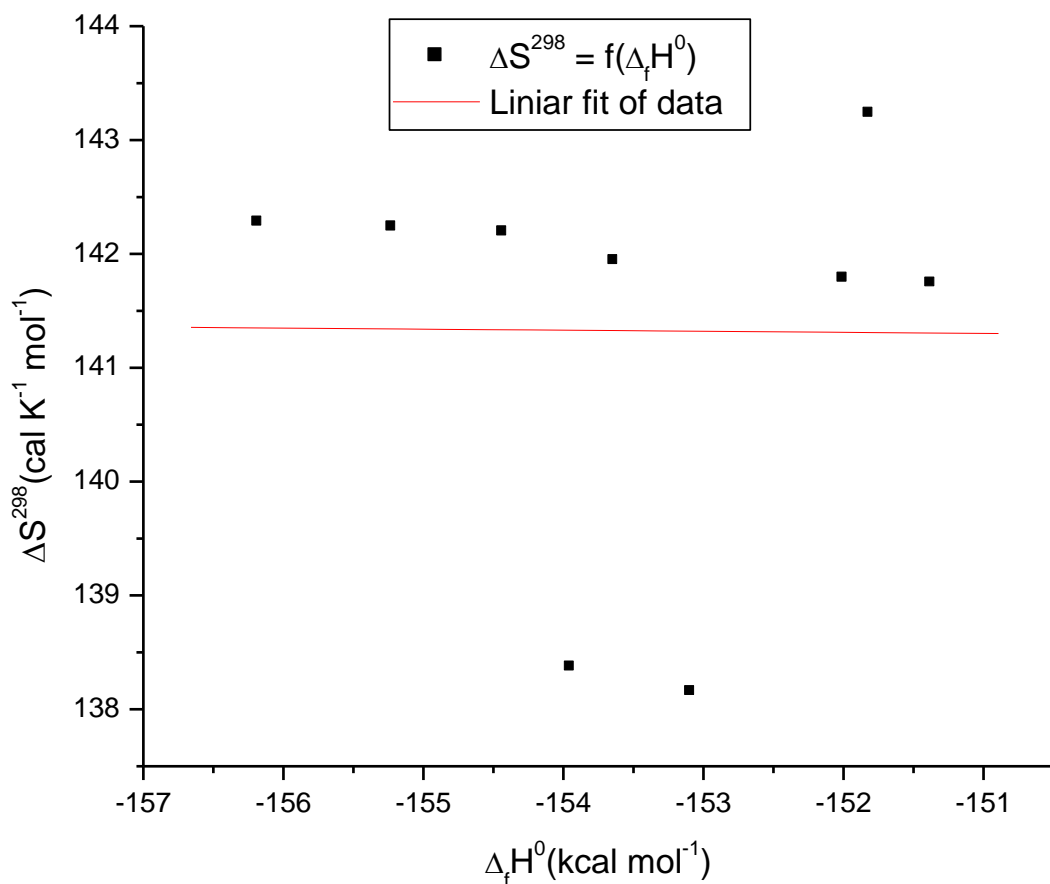


Fig. 16c. $\Delta S^0(\text{PM7}) = 139.89275 - 0.0093\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0001$; SD = 1.91541; F = 0.0001)

Table 17.
 $C_p(\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}) = f(T)$ computed by PM7-MOPAC12

Conf	PM7-01	PM7-02	PM7-03	PM7-04	PM7-05	PM7-06	PM7-07	PM7-08	PM7-09
T(K)									
100	32.2042	32.1821	31.7095	30.9587	31.6552	30.8694	32.4275	32.3671	32.1925
150	42.0364	42.0211	41.5793	41.1075	41.5485	41.0371	42.3491	42.2400	42.1278
200	51.0607	51.0601	50.6996	50.4046	50.6932	50.3608	51.3521	51.2603	51.2010
250	59.8841	59.8857	59.6224	59.4420	59.6236	59.4098	60.1474	60.0683	60.0330
298	68.3225	68.3173	68.1294	68.0226	68.1266	67.9901	68.5660	68.4879	68.4568
300	68.6715	68.6658	68.4806	68.3762	68.4775	68.3436	68.9142	68.8360	68.8048
350	77.2366	77.2213	77.0899	77.0344	77.0785	76.9971	77.4615	77.3785	77.3436
400	85.3487	85.3253	85.2290	85.2041	85.2100	85.1623	85.5556	85.4674	85.4279
450	92.8681	92.8394	92.7658	92.7597	92.7416	92.7154	93.0561	92.9649	92.9227
500	99.7505	99.7191	99.6606	99.6662	99.6336	99.6214	99.9195	99.8280	99.7853
550	106.0119	105.9798	105.9318	105.9447	105.9037	105.9009	106.1623	106.0731	106.0316
600	111.6969	111.6652	111.6250	111.6425	111.5971	111.6008	111.8297	111.7444	111.7054
650	116.8588	116.8283	116.7940	116.8147	116.7672	116.7754	116.9753	116.8952	116.8592
700	121.5502	121.5213	121.4919	121.5145	121.4664	121.4780	121.6519	121.5775	121.5450
750	125.8193	125.7922	125.7669	125.7907	125.7429	125.7569	125.9079	125.8395	125.8102
800	129.7092	129.6839	129.6621	129.6866	129.6396	129.6554	129.7861	129.7235	129.6974
850	133.2577	133.2342	133.2153	133.2402	133.1944	133.2114	133.3245	133.2674	133.2442
900	136.4984	136.4766	136.4603	136.4852	136.4408	136.4588	136.5563	136.5045	136.4839
950	139.4612	139.4409	139.4269	139.4517	139.4088	139.4273	139.5114	139.4644	139.4461
1000	142.1727	142.1538	142.1418	142.1662	142.1249	142.1437	142.2162	142.1736	142.1574

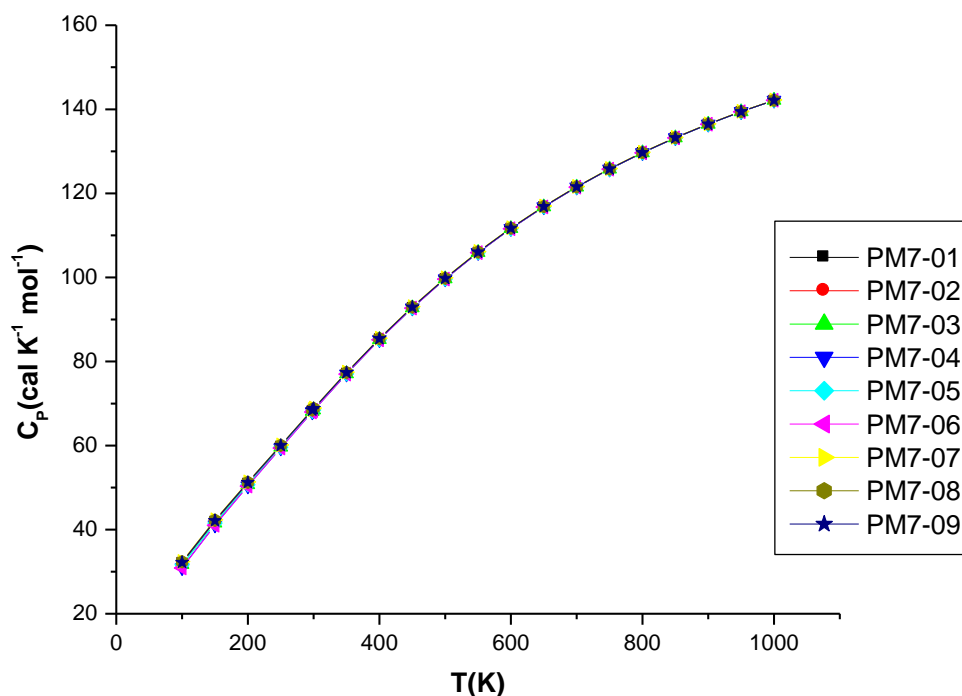


Fig. 17. Functional dependencies C_p graphs in the range of 100K-1000K resulted for conformers energetic and geometric optimized with by PM7-MOPAC12

Table 18.

MOPAC12 Polynomial interpolation relations ($y = a_0 + a_1T + a_2T^2 + a_3T^3$) of the functional dependence of $C_p(T)$ for distinct conformers with geometry optimized by the PM7 hamiltonian

Conformerul	a_0	a_1	$a_2 \cdot 10^5$	$a_3 \cdot 10^{10}$	r^2	SD	F
PM7-01	10.0525	0.2257	-9.5918	17.3891	0.9998	0.4616	35655.4
PM7-02	10.0321	0.2259	-9.6294	20.0758	0.9998	0.4547	36735.6
PM7-03	9.2778	0.2287	-9.9852	35.1858	0.9998	0.4563	36773.4
PM7-04	8.1108	0.2343	-10.8491	77.0074	0.9998	0.4263	42536.6
PM7-05	9.2044	0.2291	-10.0735	40.4202	0.9998	0.4471	38295.2
PM7-06	7.9940	0.2348	-10.9325	81.7560	0.9998	0.4182	44218.5
PM7-07	10.3049	0.2260	-9.7209	25.3778	0.9998	0.4551	36509.2
PM7-08	10.2371	0.2259	-9.7052	25.2032	0.9998	0.4515	37121.1
PM7-09	9.9897	0.2271	-9.9104	36.2541	0.9998	0.4366	39752.3
Mean	9.4670	0.2286	-10.0442	39.8522	0.9998	0.4453	38621.9
SD	0.8905	0.0036	0.5069	23.6941	0.0000	0.0149	2969.1

$$C_p(T) = 9.4670(\pm 0.8905) + 0.2286(\pm 0.0036)T - 10.0442(\pm 0.5069) \cdot 10^{-5}T^2 + 39.8522(\pm 23.6941) \cdot 10^{-10}T^3$$

$$T \in [100K, 1000K] \quad (r^2 = 0.9998; \text{SD} = 0.4453 \pm 0.0149; 38621.9(\pm 2969.1))$$

$$\Delta a_0 = 2.3109 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

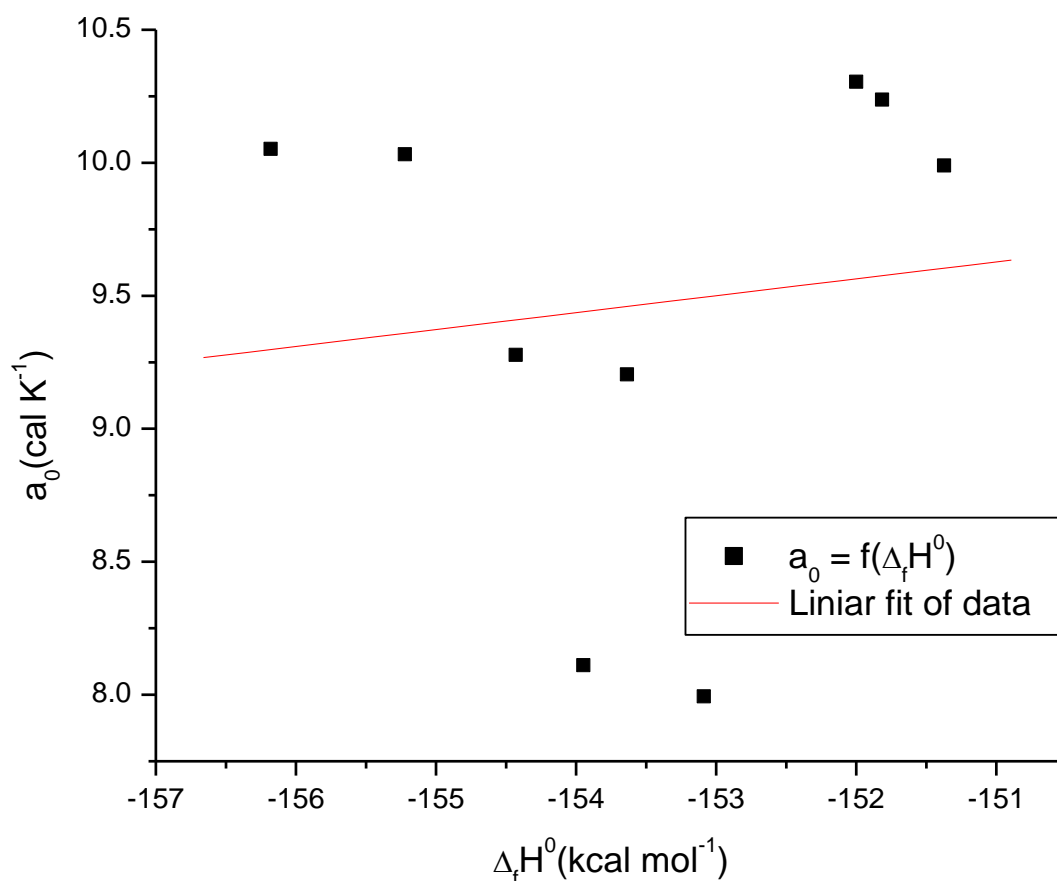


Fig. 18a. $a_0(\text{PM7}) = 19.2304 + 0.0636\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0134$; SD = 0.9456; F = 0.0950)

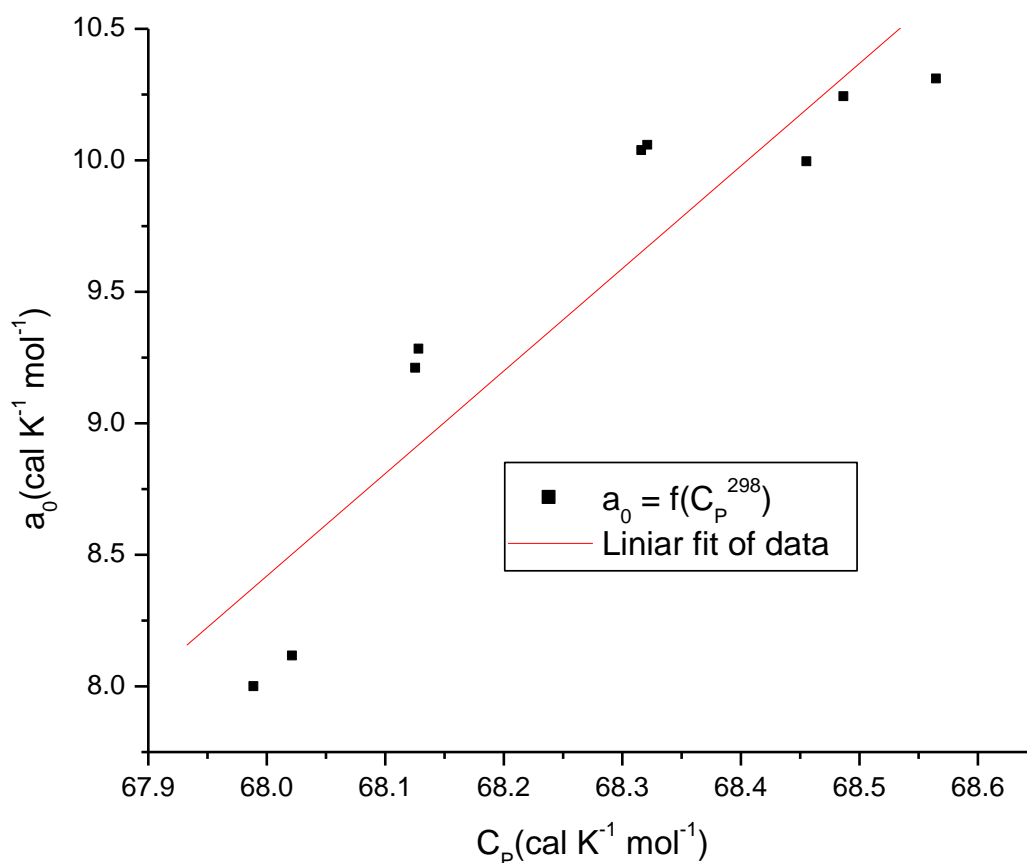


Fig. 18b. $a_0(\text{PM7}) = -256.6036 + 3.8974C_p(\text{PM7})$ ($r^2 = 0.8281$; $\text{SD} = 0.3691$; $F = 39.5448 > 1.0$)

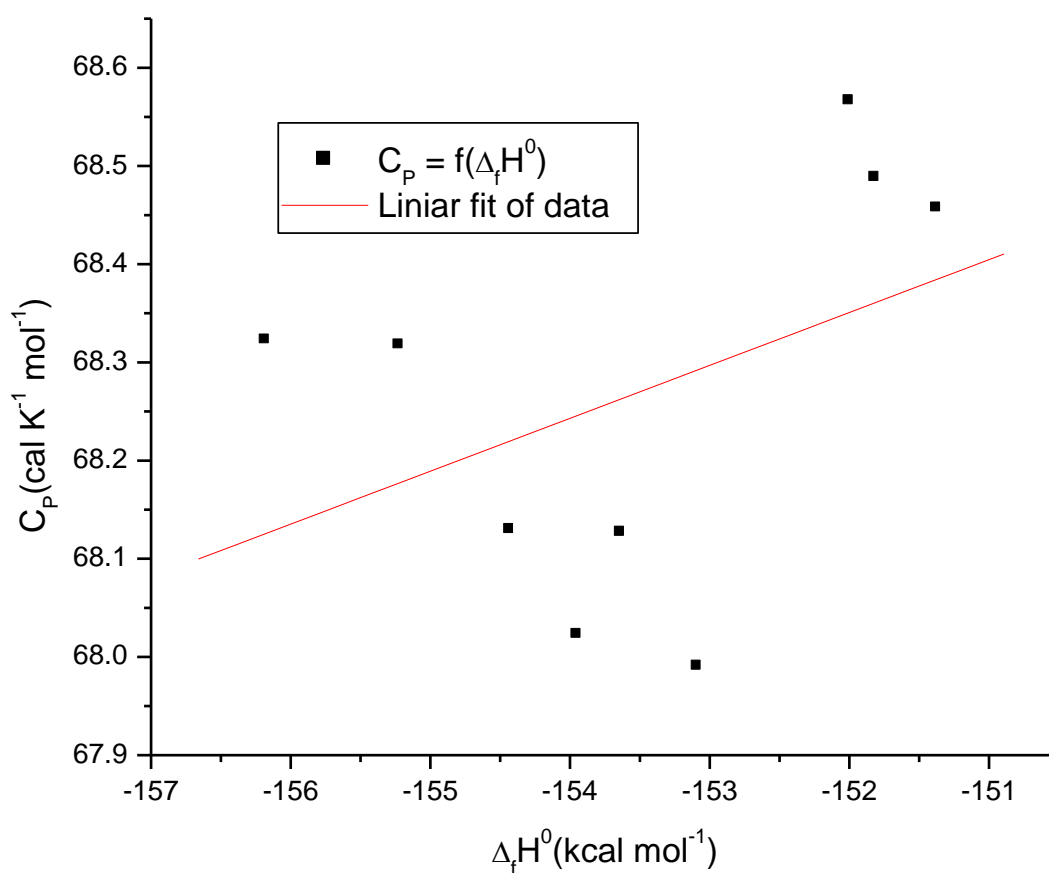


Fig. 18c. $C_p^0(\text{PM7}) = 76.5399 + 0.0539\Delta_f H^0(\text{PM7})$ ($r^2 = 0.0535$; $\text{SD} = 0.2049$; $F = 1.4526$)