Table 1: HF/STO-3G conformer ID, total energy (E_{tot}), E_{HOMO}, E_{LUMO}, μ_{TOT}, ν_0, E_{ZVP}, dihedral angles $<_d$=5-1-2-3; 5-4-3-2; 28-14-15-17, and improper dihedral angles $<_{id}$=4-5-6-7; 6-15-28-14.

ID	E_{tot}	E_{HOMO}	E_{LUMO}	μ_{TOT}	$<_d$(°)			$<_{id}$(°)		N14	17, 28	ν_0	E_{ZVP}
	kcal/mol	eV	eV	D	5-1-2-3	5-4-3-2	28-14-15-17	4-5-6-7	6-15-28-14	chir.	aran.	cm^{-1}	kcal/mol
Pn-01	-739365.587	-7.220	7.260	3.777	37.501	25.887	153.504	-0.873	-28.442	R	*anti*	32.98	179.266
Pn-02	-739365.375	-7.367	7.572	3.254	-22.107	-32.904	-153.254	-10.553	28.241	S	*anti*	33.07	179.114
Pn-03	-739365.366	-7.215	7.326	3.359	35.651	18.982	154.070	-3.824	-27.968	R	*anti*	31.49	179.232
Pn-04	-739365.305	-7.324	7.341	3.421	35.057	19.755	-150.428	-3.094	28.919	S	*anti*	24.28	179.216
Pn-05	-739365.067	-7.328	7.242	3.784	37.237	25.936	-151.196	-0.764	27.488	S	*anti*	28.34	179.191
Pn-06	-739364.826	-7.347	7.777	4.209	-19.739	-34.217	-152.064	-11.474	28.198	S	*anti*	32.03	179.134
Pn-07	-739364.609	-7.376	7.438	3.794	-22.022	-32.731	-151.889	-9.255	28.218	S	*anti*	18.30	179.063
Pn-08	-739364.609	-7.185	7.489	2.671	-20.882	-33.082	157.128	-11.786	-24.649	R	*anti*	25.93	178.989
Pn-09	-739364.173	-7.181	7.670	3.774	-18.291	-34.518	156.817	-12.812	-25.251	R	*anti*	25.29	178.984
Pn-10	-739363.927	-7.194	7.386	3.261	-21.374	-33.566	-151.579	-8.417	28.387	S	*anti*	15.47	178.924
Pn-11	-739363.920	-7.211	7.374	3.273	-21.384	-32.770	156.738	-10.229	-25.325	R	*anti*	9.52	178.931
Pn-12	-739363.626	-7.295	7.258	2.655	35.402	19.796	-14.994	-3.386	-30.490	R	*syn*	29.54	179.625
Pn-13	-739363.176	-7.354	7.359	2.515	-21.644	-33.038	-14.542	-11.176	-27.173	R	*syn*	29.81	179.379
Pn-14	-739362.993	-7.186	7.185	3.362	-20.474	-33.773	156.949	-9.442	-25.205	R	*anti*	25.25	178.996
Pn-15	-739362.932	-7.311	7.259	3.037	37.749	24.026	-16.709	-2.160	-29.914	R	*syn*	33.31	179.484
Pn-16	-739362.809	-7.345	7.517	2.725	-19.714	-34.187	-15.098	-11.860	-27.723	R	*syn*	27.28	179.353
Pn-17	-739362.683	-7.340	7.452	2.380	-21.642	-33.080	12.129	-11.105	28.663	S	*syn*	22.36	179.504
Pn-18	-739362.445	-7.360	7.276	2.824	-21.419	-32.902	-14.887	-9.848	-27.137	R	*syn*	22.06	179.363
Pn-19	-739362.267	-7.329	7.632	2.521	-19.399	-34.346	12.147	-12.002	28.669	S	*syn*	24.23	179.387
Pn-20	-739361.904	-7.338	7.338	2.689	-21.131	-32.960	12.716	-9.905	28.721	S	*syn*	20.93	179.439
Pn-21	-739361.604	-7.348	7.303	1.672	-20.873	-33.779	-14.794	-9.087	-27.290	R	*syn*	28.00	179.427
Pn-22	-739361.349	-6.797	7.976	2.518	-11.043	-33.531	-155.690	-14.306	24.177	S	*anti*	47.20	179.192
Pn-23	-739361.195	-6.815	7.811	3.116	-13.004	-32.647	-156.633	-13.853	23.347	S	*anti*	41.20	179.171
Pn-24	-739361.048	-7.331	7.361	1.528	-20.842	-33.714	12.621	-8.992	28.797	S	*syn*	16.66	179.428
Pn-25	-739360.798	-6.801	7.766	2.580	-7.270	-29.081	-153.878	-11.617	25.197	S	*anti*	26.55	179.175
Pn-26	-739360.188	-6.796	7.737	2.996	-6.985	-29.542	-153.626	-10.900	25.173	S	*anti*	28.04	179.254
Pn-27	-739356.710	-7.271	7.328	2.765	32.691	0.107	7.910	-13.194	24.905	S	*syn*	43.39	179.526
Pn-28	-739356.653	-7.280	7.384	3.619	33.118	2.275	7.559	-11.708	27.782	S	*syn*	30.09	179.558
Mean		**-7.223**	**7.458**	**3.003**				**-9.201**				**27.59**	**179.261**
SD		0.186	0.207	0.627				3.947				8.12	0.200

Table 2. ΔH_{form}(kcal/mol) = f(T) computed by PM6-MOPAC12.*

ID T	1	2	3	4	5	6	7	8	9	10	11	12	13	14
200	-172.925	-172.823	-171.926	-171.758	-171.508	-171.455	-170.645	-170.306	-169.870	-169.699	-168.944	-168.877	-168.695	-168.435
210	-172.408	-172.305	-171.407	-171.241	-170.990	-170.938	-170.127	-169.790	-169.354	-169.183	-168.428	-168.368	-168.178	-167.927
220	-171.873	-171.768	-170.869	-170.705	-170.454	-170.403	-169.590	-169.255	-168.820	-168.649	-167.893	-167.840	-167.643	-167.401
230	-171.321	-171.214	-170.314	-170.151	-169.900	-169.849	-169.035	-168.701	-168.268	-168.097	-167.340	-167.294	-167.090	-166.857
240	-170.750	-170.641	-169.740	-169.579	-169.328	-169.277	-168.462	-168.130	-167.698	-167.527	-166.769	-166.729	-166.518	-166.293
250	-170.161	-170.050	-169.149	-168.989	-168.738	-168.687	-167.871	-167.540	-167.109	-166.938	-166.179	-166.145	-165.928	-165.711
260	-169.553	-169.442	-168.539	-168.380	-168.129	-168.079	-167.262	-166.931	-166.503	-166.331	-165.571	-165.543	-165.320	-165.110
270	-168.928	-168.815	-167.911	-167.754	-167.502	-167.453	-166.634	-166.305	-165.878	-165.706	-164.945	-164.922	-164.694	-164.490
280	-168.285	-168.169	-167.265	-167.109	-166.857	-166.808	-165.989	-165.660	-165.234	-165.063	-164.301	-164.283	-164.049	-163.852
290	-167.623	-167.506	-166.601	-166.446	-166.194	-166.146	-165.325	-164.997	-164.573	-164.401	-163.638	-163.625	-163.386	-163.195
298	-167.080	-166.963	-166.057	-165.903	-165.650	-165.603	-164.781	-164.453	-164.031	-163.859	-163.095	-163.086	-162.843	-162.656
300	-166.943	-166.825	-165.919	-165.765	-165.512	-165.465	-164.643	-164.315	-163.893	-163.721	-162.958	-162.949	-162.705	-162.519
310	-166.245	-166.126	-165.219	-165.066	-164.813	-164.766	-163.944	-163.616	-163.196	-163.023	-162.259	-162.255	-162.006	-161.826
320	-165.529	-165.409	-164.501	-164.349	-164.096	-164.050	-163.226	-162.899	-162.480	-162.308	-161.542	-161.542	-161.289	-161.114
330	-164.796	-164.674	-163.766	-163.615	-163.361	-163.315	-162.491	-162.164	-161.747	-161.574	-160.808	-160.812	-160.555	-160.384
340	-164.045	-163.922	-163.013	-162.863	-162.608	-162.563	-161.738	-161.412	-160.996	-160.823	-160.056	-160.063	-159.803	-159.637
350	-163.276	-163.152	-162.243	-162.093	-161.838	-161.794	-160.968	-160.642	-160.228	-160.055	-159.287	-159.298	-159.033	-158.872
360	-162.490	-162.366	-161.455	-161.307	-161.051	-161.008	-160.181	-159.855	-159.442	-159.269	-158.500	-158.515	-158.246	-158.089
370	-161.687	-161.562	-160.651	-160.503	-160.247	-160.204	-159.377	-159.051	-158.640	-158.467	-157.697	-157.714	-157.442	-157.289
380	-160.868	-160.742	-159.830	-159.683	-159.426	-159.384	-158.556	-158.230	-157.821	-157.647	-156.876	-156.897	-156.622	-156.473
390	-160.032	-159.905	-158.993	-158.846	-158.589	-158.54	-157.719	-157.393	-156.985	-156.811	-156.039	-156.063	-155.785	-155.639
400	-159.179	-159.052	-158.139	-157.993	-157.736	-157.695	-156.865	-156.540	-156.133	-155.959	-155.186	-155.213	-154.931	-154.790

*: NOTE: Heats of Formation are relative to the elements in their standard state at 298K = Standard Enthalpy of Formation.
H_{vib}: Zero-point energy is not included. Frequencies of less than zero cm^{-1} are not included.
$H_{rot} = (3/2)RT$
$H_{tra} = (3/2)RT + pV = (5/2)RT$

Table 3. ΔH_{form}(kcal/mol) = f(T) computed by PM7-MOPAC12.*

ID T	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
200	-161.978	-160.253	-158.918	-158.907	-158.606	-158.508	-157.797	-157.528	-157.062	-156.851	-156.788	-156.683	-156.579	-156.218	-156.045	-155.819	-155.764	-155.243	-154.940
210	-161.469	-159.745	-158.407	-158.394	-158.100	-157.995	-157.291	-157.014	-156.551	-156.339	-156.279	-156.171	-156.069	-155.707	-155.534	-155.306	-155.251	-154.738	-154.434
220	-160.943	-159.218	-157.877	-157.863	-157.576	-157.463	-156.767	-156.481	-156.022	-155.808	-155.752	-155.640	-155.541	-155.177	-155.005	-154.775	-154.720	-154.215	-153.910
230	-160.399	-158.674	-157.329	-157.315	-157.033	-156.913	-156.225	-155.931	-155.475	-155.260	-155.207	-155.092	-154.994	-154.629	-154.458	-154.226	-154.170	-153.673	-153.368
240	-159.836	-158.111	-156.763	-156.748	-156.472	-156.346	-155.664	-155.362	-154.910	-154.693	-154.643	-154.525	-154.430	-154.063	-153.892	-153.658	-153.603	-153.113	-152.807
250	-159.256	-157.530	-156.178	-156.163	-155.894	-155.760	-155.086	-154.776	-154.327	-154.108	-154.061	-153.940	-153.847	-153.478	-153.308	-153.073	-153.017	-152.535	-152.228
260	-158.658	-156.931	-155.576	-155.561	-155.297	-155.157	-154.489	-154.172	-153.725	-153.506	-153.462	-153.337	-153.247	-152.876	-152.707	-152.470	-152.414	-151.938	-151.630
270	-158.04	-156.314	-154.956	-154.940	-154.682	-154.536	-153.874	-153.550	-153.106	-152.886	-152.844	-152.717	-152.628	-152.256	-152.087	-151.849	-151.792	-151.323	-151.014
280	-157.407	-155.679	-154.318	-154.302	-154.049	-153.897	-153.240	-152.910	-152.468	-152.247	-152.208	-152.078	-151.992	-151.618	-151.449	-151.209	-151.153	-150.690	-150.380
290	-156.755	-155.026	-153.662	-153.646	-153.399	-153.240	-152.589	-152.252	-151.813	-151.591	-151.554	-151.422	-151.338	-150.961	-150.793	-150.552	-150.496	-150.038	-149.728
298	-156.221	-154.491	-153.125	-153.108	-152.865	-152.702	-152.055	-151.713	-151.276	-151.053	-151.018	-150.884	-150.802	-150.424	-150.255	-150.014	-149.957	-149.504	-149.194
300	-156.085	-154.355	-152.989	-152.972	-152.730	-152.565	-151.920	-151.577	-151.140	-150.917	-150.882	-150.747	-150.666	-150.288	-150.119	-149.878	-149.821	-149.369	-149.058
310	-155.397	-153.667	-152.298	-152.281	-152.044	-151.873	-151.233	-150.884	-150.449	-150.226	-150.193	-150.055	-149.976	-149.596	-149.428	-149.185	-149.128	-148.682	-148.370
320	-154.692	-152.961	-151.589	-151.572	-151.340	-151.163	-150.528	-150.173	-149.741	-149.517	-149.486	-149.346	-149.268	-148.887	-148.719	-148.475	-148.418	-147.977	-147.664
330	-153.969	-152.237	-150.863	-150.845	-150.618	-150.436	-149.806	-149.445	-149.015	-148.790	-148.761	-148.619	-148.544	-148.160	-147.992	-147.748	-147.691	-147.254	-146.941
340	-153.229	-151.496	-150.120	-150.102	-149.879	-149.692	-149.066	-148.700	-148.272	-148.047	-148.019	-147.875	-147.801	-147.416	-147.248	-147.004	-146.946	-146.514	-146.201
350	-152.471	-150.738	-149.359	-149.341	-149.123	-148.931	-148.309	-147.938	-147.512	-147.286	-147.260	-147.114	-147.042	-146.655	-146.488	-146.242	-146.184	-145.757	-145.443
360	-151.697	-149.962	-148.582	-148.564	-148.350	-148.153	-147.535	-147.159	-146.735	-146.509	-146.485	-146.337	-146.266	-145.878	-145.710	-145.463	-145.405	-144.982	-144.668
370	-150.906	-149.170	-147.788	-147.770	-147.561	-147.358	-146.745	-146.364	-145.941	-145.714	-145.692	-145.542	-145.473	-145.083	-144.915	-144.668	-144.610	-144.191	-143.876
380	-150.098	-148.362	-146.977	-146.959	-146.754	-146.547	-145.937	-145.552	-145.131	-144.904	-144.883	-144.731	-144.664	-144.272	-144.104	-143.857	-143.798	-143.383	-143.068
390	-149.274	-147.537	-146.151	-146.133	-145.932	-145.720	-145.113	-144.723	-144.305	-144.077	-144.057	-143.904	-143.838	-143.445	-143.277	-143.029	-142.970	-142.559	-142.243
400	-148.434	-146.696	-145.308	-145.290	-145.093	-144.876	-144.274	-143.879	-143.462	-143.234	-143.216	-143.061	-142.996	-142.602	-142.434	-142.185	-142.126	-141.719	-141.403

*: NOTE: Heats of Formation are relative to the elements in their standard state at 298K = Standard Enthalpy of Formation.
H_{vib}: Zero-point energy is not included. Frequencies of less than zero cm^{-1} are not included.
$H_{rot} = (3/2)RT$
$H_{tra} = (3/2)RT + pV = (5/2)RT$

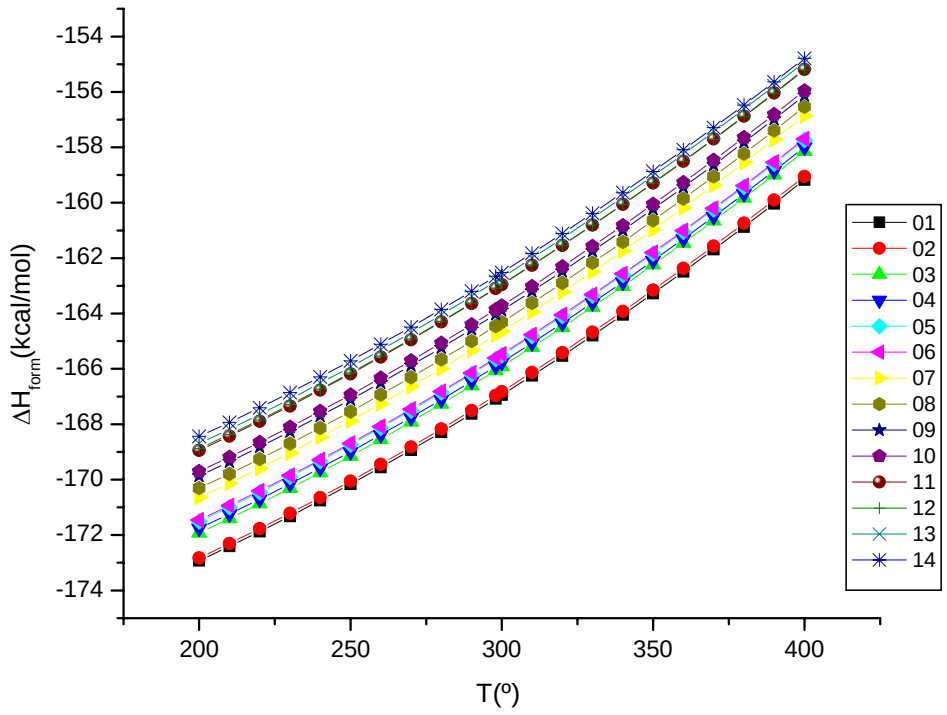

Figure 1. Plots of the functional dependence of ΔH_{form} on T in the temperature range: 200-400K for the 14 conformers derived from PM6 optimization.

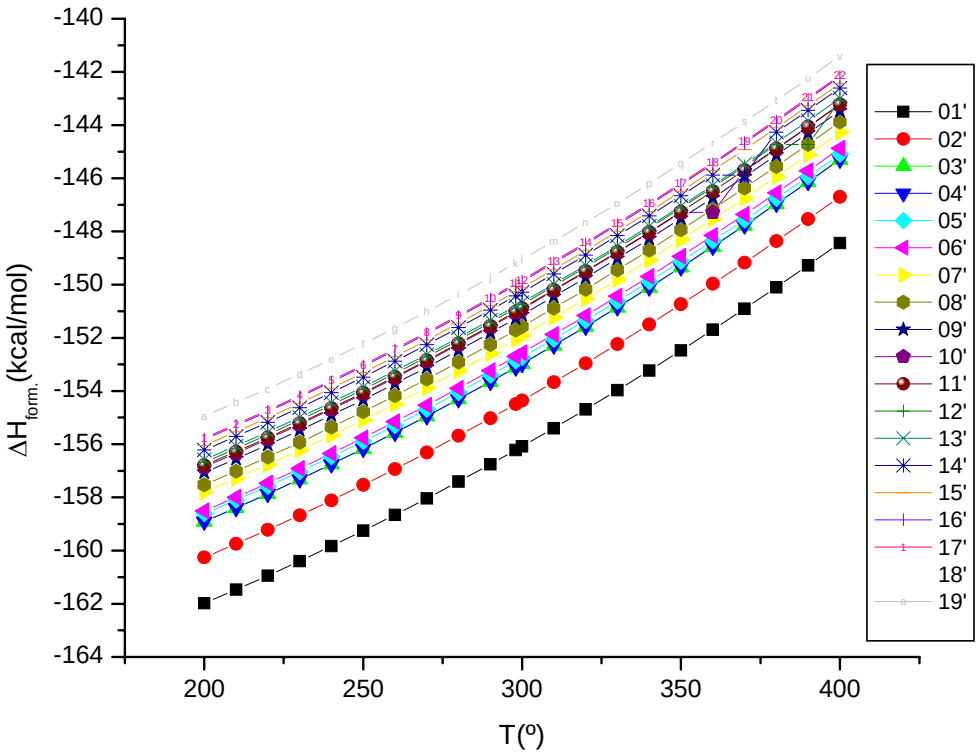

Figure 2. Plots of the functional dependence of ΔH_{form} on T in the temperature range: 200-400K for the 19 conformers derived from PM7 optimization.