DFT Calculation on 76 Polybromophenazines: Their Thermodynamic Function and Stability[†]. Ping Sun, Guo Y. Yang, Hong X. Liu, and Zun Y. Wang,* *J. Chem. Eng. Data* **2009,** *54,* 2404–2410.

Molecular symmetry and vibrational scaling factors were not accounted for in the calculations. Tables 4a (pages 2406 to 2407) and 6a (page 2408) below result from a recalculation at the B3LYP/6-31G* level with a vibrational scaling factor of 0.96 and with the symmetry numbers given in the tables.

Table 4a. Thermodynamic Parameters by B3LYP/6-31G* for PBPZs[a]

			$S^{\ominus}$	$\Delta_f H^{\ominus}$	$\Delta_f G^{\ominus}$	$\Delta_f G_R^{\ominus}$	$C_{p,m}$/J·mol^{-1}·K^{-1}									
molecule	group	symmetry number	J·mol^{-1}·K^{-1}	kJ·mol^{-1}	kJ·mol^{-1}	kJ·mol^{-1}	constant	$10^{-3}T$	$10^{5}T^{-1}$	$10^{7}T^{-2}$	N_α	N_β	N_o	N_m	N_p	$N_{1,9}$
PZ	D_{2H}	4	387.192	343.600	243.300		517.843	39.320	−1.510	1.384	0	0	0	0	0	0
MBPZ																
1-MBPZ	C_S	1	439.638	373.789	417.248	5.758	529.798	32.554	−1.474	1.339	1	0	0	0	0	0
2-MBPZ	C_S	1	440.776	368.370	411.490	0.000	529.701	32.350	−1.469	1.331	0	1	0	0	0	0
DBPZ																
1,2-DBPZ	C_S	1	479.541	406.404	441.763	11.828	541.959	25.601	−1.437	1.291	1	1	1	0	0	0
1,3-DBPZ	C_S	1	482.076	401.224	435.827	5.892	541.931	25.464	−1.435	1.289	1	1	0	1	0	0
1,4-DBPZ	C_{2V}	2	474.838	405.769	442.530	12.595	541.670	25.909	−1.439	1.296	2	0	0	0	1	0
1,6-DBPZ	C_{2H}	2	475.189	404.475	441.131	11.195	541.744	25.802	−1.439	1.294	2	0	0	0	0	0
1,7-DBPZ	C_S	1	482.244	399.431	433.981	4.046	541.625	25.604	−1.433	1.285	1	1	0	0	0	0
1,8-DBPZ	C_S	1	481.608	399.449	434.191	4.256	541.677	25.569	−1.433	1.286	1	1	0	0	0	0
1,9-DBPZ	C_{2V}	2	475.076	405.863	442.551	12.616	541.699	25.832	−1.438	1.294	2	0	0	0	0	1
2,3-DBPZ	C_{2V}	2	474.265	403.521	440.453	10.518	542.022	25.371	−1.433	1.285	0	2	1	0	0	0
2,7-DBPZ	C_{2H}	2	477.286	393.999	430.030	0.095	541.505	25.435	−1.428	1.278	0	2	0	0	0	0
2,8-DBPZ	C_{2V}	2	477.294	393.907	429.936	0.000	541.625	25.346	−1.428	1.278	0	2	0	0	0	0
tri-BPZ																
1,2,3-tri-BPZ	C_S	1	518.665	445.132	472.622	19.148	554.844	18.276	−1.403	1.246	1	2	2	1	0	0
1,2,4-tri-BPZ	C_S	1	520.577	440.435	467.355	13.881	554.254	18.761	−1.405	1.252	2	1	1	1	1	0
1,2,6-tri-BPZ	C_S	1	520.557	437.631	464.556	11.082	553.929	18.840	−1.401	1.246	2	1	1	0	0	0
1,2,7-tri-BPZ	C_S	1	520.690	432.461	459.347	5.873	553.877	18.645	−1.397	1.238	1	2	1	0	0	0
1,2,8-tri-BPZ	C_S	1	521.724	432.621	459.200	5.726	553.904	18.609	−1.396	1.238	1	2	1	0	0	0
1,2,9-tri-BPZ	C_S	1	520.322	438.891	465.885	12.411	553.908	18.882	−1.402	1.246	2	1	1	0	0	1
1,3,6-tri-BPZ	C_S	1	522.414	432.863	459.232	5.758	553.848	18.767	−1.400	1.245	2	1	0	1	0	0
1,3,7-tri-BPZ	C_S	1	523.117	427.318	453.482	0.008	553.808	18.536	−1.395	1.237	1	2	0	1	0	0
1,3,8-tri-BPZ	C_S	1	523.808	427.517	453.474	0.000	553.761	18.552	−1.394	1.236	1	2	0	1	0	0
1,3,9-tri-BPZ	C_S	1	522.715	433.913	460.195	6.721	553.837	18.771	−1.399	1.244	2	1	0	1	0	1
1,4,6-tri-BPZ	C_S	1	521.594	438.518	465.134	11.660	553.600	19.189	−1.404	1.251	3	0	0	0	1	1
1,4,7-tri-BPZ	C_S	1	523.042	432.254	458.436	4.962	553.524	18.964	−1.398	1.242	2	1	0	0	1	0
2,3,6-tri-BPZ	C_S	1	521.251	435.283	462.002	8.528	554.027	18.573	−1.397	1.239	1	2	1	0	0	0
2,3,7-tri-BPZ	C_S	1	522.431	429.799	456.165	2.691	553.831	18.462	−1.392	1.230	0	3	1	0	0	0
TBPZ																
1,2,3,4-TBPZ	C_{2V}	2	551.384	488.264	509.795	28.686	567.852	11.138	−1.374	1.211	2	2	3	2	1	0
1,2,3,6-TBPZ	C_S	1	559.761	477.140	496.174	15.065	566.854	11.509	−1.367	1.201	2	2	2	1	0	0
1,2,3,7-TBPZ	C_S	1	560.610	471.574	490.353	9.244	566.792	11.297	−1.362	1.194	1	3	2	1	0	0
1,2,3,8-TBPZ	C_S	1	560.920	471.834	490.521	9.412	566.827	11.264	−1.362	1.194	1	3	2	1	0	0
1,2,3,9-TBPZ	C_S	1	560.058	478.067	497.011	15.903	566.919	11.476	−1.368	1.202	2	2	2	1	0	1
1,2,4,6-TBPZ	C_S	1	561.480	473.341	491.863	10.754	566.124	12.107	−1.369	1.208	3	1	1	1	1	1
1,2,4,7-TBPZ	C_S	1	562.267	467.284	485.572	4.463	566.028	11.904	−1.364	1.199	2	2	1	1	1	0
1,2,4,8-TBPZ	C_S	1	562.095	467.200	485.538	4.429	566.084	11.859	−1.364	1.199	2	2	1	1	1	0
1,2,4,9-TBPZ	C_S	1	561.300	473.504	492.078	10.969	566.235	12.048	−1.370	1.208	3	1	1	1	1	1
1,2,6,7-TBPZ	C_{2H}	2	553.476	471.104	492.010	10.901	566.187	11.882	−1.366	1.199	2	2	2	0	0	0
1,2,6,8-TBPZ	C_S	1	562.685	466.412	484.574	3.466	566.159	11.742	−1.363	1.197	2	2	1	1	0	0
1,2,6,9-TBPZ	C_S	1	561.593	471.894	490.379	9.271	565.837	12.226	−1.367	1.204	3	1	1	0	1	1
1,2,7,8-TBPZ	C_S	1	560.823	468.586	487.302	6.194	566.268	11.617	−1.361	1.191	1	3	2	0	0	0
1,2,7,9-TBPZ	C_S	1	562.857	467.355	485.464	4.356	566.034	11.826	−1.362	1.196	2	2	1	1	0	1
1,2,8,9-TBPZ	C_{2V}	2	554.882	472.141	492.629	11.521	566.112	11.914	−1.365	1.198	2	2	2	0	0	1
1,3,6,8-TBPZ	C_{2H}	2	559.074	461.870	481.109	0.000	566.000	11.733	−1.361	1.196	2	2	0	2	0	0
1,3,6,9-TBPZ	C_S	1	563.660	463.908	481.778	0.670	565.886	12.074	−1.366	1.203	3	1	0	1	1	1
1,3,7,8-TBPZ	C_S	1	563.660	463.908	481.778	0.670	566.198	11.518	−1.359	1.189	1	3	1	1	0	0
1,3,7,9-TBPZ	C_{2V}	2	559.112	462.498	481.723	0.614	566.108	11.657	−1.361	1.195	2	2	0	2	0	1
1,4,6,9-TBPZ	D_{2H}	4	551.154	472.782	494.381	13.272	565.631	12.530	−1.371	1.210	4	0	0	0	2	2
1,4,7,8-TBPZ	C_{2V}	2	555.874	468.626	488.817	7.708	565.991	11.937	−1.364	1.197	2	2	1	0	1	0
2,3,7,8-TBPZ	D_{2H}	4	549.451	465.643	487.749	6.640	566.258	11.449	−1.357	1.185	0	4	2	0	0	0

Table 4a. Continued

molecule	group	symmetry number	S^{Θ} J·mol^{-1}·K^{-1}	$\Delta_f H^{\Theta}$ kJ·mol^{-1}	$\Delta_f G^{\Theta}$ kJ·mol^{-1}	$\Delta_f G_R^{\Theta}$ kJ·mol^{-1}	$C_{p,m}$/J·mol^{-1}·K^{-1} constant	$10^{-3}T$	$10^{5}T^{-1}$	$10^{7}T^{-2}$	N_α	N_β	N_o	N_m	N_p	$N_{1,9}$
penta-BPZ																
1,2,3,4,6-penta-BPZ	C_S	1	597.906	521.460	532.916	20.665	579.948	4.330	−1.339	1.167	3	2	3	2	1	1
1,2,3,4,7-penta-BPZ	C_S	1	599.433	515.366	526.368	14.117	579.938	4.061	−1.334	1.158	2	3	3	2	1	0
1,2,3,6,7-penta-BPZ	C_S	1	598.898	510.624	521.787	9.536	579.229	4.473	−1.332	1.155	2	3	3	1	0	0
1,2,3,6,8-penta-BPZ	C_S	1	601.513	506.059	516.438	4.188	579.093	4.419	−1.329	1.153	2	3	2	2	0	0
1,2,3,6,9-penta-BPZ	C_S	1	601.061	511.612	522.125	9.875	578.967	4.762	−1.334	1.160	3	2	2	1	1	1
1,2,3,7,8-penta-BPZ	C_S	1	600.069	508.172	518.985	6.734	579.365	4.187	−1.328	1.148	1	4	3	1	0	0
1,2,3,7,9-penta-BPZ	C_S	1	601.609	506.936	517.289	5.038	579.178	4.363	−1.329	1.153	2	3	2	2	0	1
1,2,3,8,9-penta-BPZ	C_S	1	599.500	511.627	522.608	10.358	579.138	4.530	−1.331	1.154	2	3	3	1	0	1
1,2,4,6,7-penta-BPZ	C_S	1	601.960	507.130	517.378	5.128	578.446	5.082	−1.333	1.160	3	2	2	1	1	1
1,2,4,6,8-penta-BPZ	C_S	1	603.630	502.501	512.251	0.000	578.410	4.964	−1.330	1.158	3	2	1	2	1	1
1,2,4,6,9-penta-BPZ	C_S	1	603.329	507.988	517.827	5.577	578.260	5.335	−1.336	1.166	4	1	1	1	2	2
1,2,4,7,8-penta-BPZ	C_S	1	601.312	503.832	514.272	2.022	578.620	4.766	−1.329	1.153	2	3	2	1	1	0
1,2,4,7,9-penta-BPZ	C_S	1	603.073	502.525	512.442	0.192	578.320	5.045	−1.331	1.159	3	2	1	2	1	1
1,2,4,8,9-penta-BPZ	C_S	1	600.889	507.051	517.617	5.367	578.478	5.067	−1.333	1.160	3	2	2	1	1	1
hexa-BPZ																
1,2,3,4,6,7-hexa-BPZ	C_S	1	637.399	555.301	558.781	11.783	592.315	−2.707	−1.303	1.120	3	3	4	2	1	1
1,2,3,4,6,8-hexa-BPZ	C_S	1	639.838	550.809	553.561	6.564	592.277	−2.821	−1.301	1.118	3	3	3	3	1	1
1,2,3,4,6,9-hexa-BPZ	C_{2V}	2	633.441	556.070	560.729	13.731	591.979	−2.331	−1.306	1.125	4	2	3	2	2	2
1,2,3,4,7,8-hexa-BPZ	C_{2V}	2	632.374	552.074	557.051	10.053	592.349	−2.938	−1.299	1.112	2	4	4	2	1	0
1,2,3,6,7,8-hexa-BPZ	C_{2H}	2	632.537	550.612	555.541	8.543	592.248	−2.909	−1.298	1.111	2	4	4	2	0	0
1,2,3,6,7,9-hexa-BPZ	C_S	1	640.144	546.968	549.628	2.631	591.589	−2.365	−1.300	1.117	3	3	3	2	1	1
1,2,3,6,8,9-hexa-BPZ	C_S	1	639.763	546.886	549.660	2.662	591.553	−2.347	−1.300	1.117	3	3	3	2	1	1
1,2,3,7,8,9-hexa-BPZ	C_{2V}	2	632.575	551.082	555.998	9.000	592.182	−2.871	−1.298	1.111	2	4	4	2	0	1
1,2,4,6,7,9-hexa-BPZ	C_{2H}	2	634.412	543.216	547.586	0.588	590.756	−1.664	−1.303	1.124	4	2	2	2	2	2
1,2,4,6,8,9-hexa-BPZ	C_{2V}	2	636.349	543.205	546.998	0.000	590.745	−1.686	−1.301	1.123	4	2	2	2	2	2
hepta-BPZ																
1,2,3,4,6,7,8-hepta-BPZ	C_S	1	677.904	595.268	590.467	4.135	605.334	−10.099	−1.269	1.075	3	4	5	3	1	1
1,2,3,4,6,7,9-hepta-BPZ	C_S	1	679.754	591.684	586.331	0.000	604.560	−9.469	−1.271	1.081	4	3	4	3	2	2
OBPZ																
1,2,3,4,6,7,8,9-OBPZ	D_{2H}	4	704.075	639.653	630.845	0.268	618.328	−17.207	−1.241	1.04	4	4	6	4	2	2

[a] S^{Θ} is standard entropy; $\Delta_f H^{\Theta}$ is the standard enthalpy of formation of the compound; $\Delta_f G^{\Theta}$ is the standard Gibbs energy of formation of the compound; and $\Delta_f G_R^{\Theta}$ is the relative magnitude of the standard Gibbs energy of formation; $C_{p,m}^{\Theta}$ is molar heat capacity at constant pressure. N is the number of Br atom substitutions, and the subscript PBS indicates the positions.

Table 6a. Molar Heat Capacity at Constant Pressure for (200 to 1000) K

	$C_{p,m}$/J·mol^{-1}·K^{-1}								
	T/K								
	200	300	400	500	600	700	800	900	1000
PZ	116.64	181.55	241.24	290.03	328.43	358.72	383.00	402.79	419.13
MBPZ									
1-MBPZ	133.78	198.32	256.62	303.96	341.02	370.11	393.28	412.05	427.47
2-MBPZ	134.31	199.03	257.29	304.51	341.47	370.45	393.55	412.26	427.63
DBPZ									
1,2-DBPZ	151.15	215.42	272.35	318.19	353.89	381.72	403.75	421.48	435.96
1,3-DBPZ	151.76	215.88	272.71	318.47	354.09	381.87	403.85	421.55	436.00
1,4-DBPZ	150.94	214.97	271.85	317.75	353.51	381.40	403.48	421.25	435.77
1,6-DBPZ	150.88	215.04	271.95	317.84	353.59	381.46	403.53	421.29	435.79
1,7-DBPZ	151.49	215.85	272.71	318.48	354.10	381.87	403.85	421.54	436.00
1,8-DBPZ	151.39	215.77	272.65	318.43	354.06	381.83	403.82	421.51	435.97
1,9-DBPZ	150.89	215.05	271.96	317.85	353.59	381.47	403.53	421.29	435.80
2,3-DBPZ	151.29	215.83	272.78	318.58	354.20	381.97	403.94	421.63	436.08
2,7-DBPZ	151.98	216.50	273.32	318.98	354.50	382.18	404.09	421.73	436.14
2,8-DBPZ	151.92	216.48	273.32	318.99	354.51	382.19	404.09	421.73	436.14
tri-BPZ									
1,2,3-tri-BPZ	168.55	232.51	288.12	332.51	366.84	393.43	414.32	431.00	444.54
1,2,4-tri-BPZ	168.56	232.10	287.59	332.00	366.39	393.04	413.98	430.71	444.29
1,2,6-tri-BPZ	168.23	232.15	287.70	332.10	366.47	393.10	414.02	430.74	444.30
1,2,7-tri-BPZ	168.60	232.74	288.27	332.59	366.86	393.41	414.26	430.93	444.45
1,2,8-tri-BPZ	168.75	232.87	288.38	332.68	366.94	393.47	414.32	430.97	444.49
1,2,9-tri-BPZ	168.17	232.09	287.65	332.06	366.44	393.08	414.00	430.73	444.30
1,3,6-tri-BPZ	168.73	232.49	287.95	332.28	366.60	393.18	414.07	430.76	444.31
1,3,7-tri-BPZ	169.14	233.14	288.58	332.82	367.03	393.52	414.33	430.97	444.47
1,3,8-tri-BPZ	169.30	233.27	288.69	332.90	367.10	393.58	414.38	431.01	444.51
1,3,9-tri-BPZ	168.75	232.53	287.99	332.32	366.63	393.21	414.09	430.79	444.33
1,4,6-tri-BPZ	168.04	231.69	287.19	331.64	366.08	392.77	413.74	430.51	444.11
1,4,7-tri-BPZ	168.60	232.46	287.92	332.25	366.57	393.16	414.05	430.75	444.30
2,3,6-tri-BPZ	168.49	232.68	288.25	332.58	366.87	393.42	414.27	430.94	444.47
2,3,7-tri-BPZ	169.00	233.39	288.91	333.14	367.31	393.77	414.56	431.17	444.65

Table 6a. Continued

	$C_{p,m}$/J·mol^{-1}·K^{-1}								
	T/K								
	200	300	400	500	600	700	800	900	1000
TBPZ									
1,2,3,4-TBPZ	185.62	248.97	303.26	346.30	379.37	404.80	424.62	440.32	452.96
1,2,3,6-TBPZ	185.60	249.21	303.45	346.41	379.42	404.80	424.59	440.26	452.89
1,2,3,7-TBPZ	186.05	249.87	304.09	346.94	379.85	405.14	424.85	440.47	453.05
1,2,3,8-TBPZ	186.11	249.92	304.13	346.98	379.88	405.16	424.87	440.49	453.06
1,2,3,9-TBPZ	185.63	249.24	303.48	346.44	379.45	404.83	424.61	440.29	452.91
1,2,4,6-TBPZ	185.55	248.72	302.84	345.82	378.9	404.36	424.2	439.94	452.61
1,2,4,7-TBPZ	186.05	249.45	303.53	346.4	379.37	404.73	424.5	440.17	452.79
1,2,4,8-TBPZ	186.04	249.46	303.55	346.43	379.39	404.74	424.51	440.18	452.80
1,2,4,9-TBPZ	185.55	248.73	302.86	345.84	378.93	404.38	424.23	439.96	452.63
1,2,6,7-TBPZ	185.36	249.03	303.25	346.20	379.23	404.62	424.42	440.12	452.75
1,2,6,8-TBPZ	186.08	249.59	303.70	346.55	379.49	404.83	424.57	440.23	452.83
1,2,6,9-TBPZ	185.33	248.72	302.87	345.85	378.92	404.37	424.21	439.94	452.61
1,2,7,8-TBPZ	185.70	249.65	303.88	346.75	379.68	404.99	424.72	440.36	452.95
1,2,7,9-TBPZ	186.05	249.58	303.68	346.53	379.48	404.82	424.56	440.22	452.83
1,2,8,9-TBPZ	185.50	249.17	303.37	346.30	379.31	404.69	424.48	440.17	452.80
1,3,6,8-TBPZ	186.56	249.93	303.94	346.73	379.62	404.91	424.63	440.26	452.85
1,3,6,9-TBPZ	185.83	249.09	303.16	346.07	379.09	404.49	424.30	440.00	452.64
1,3,7,8-TBPZ	186.34	250.14	304.26	347.04	379.90	405.16	424.84	440.44	453.01
1,3,7,9-TBPZ	186.56	249.96	303.99	346.77	379.66	404.95	424.66	440.29	452.87
1,4,6,9-TBPZ	185.11	248.22	302.33	345.36	378.52	404.04	423.94	439.72	452.42
1,4,7,8-TBPZ	185.48	249.19	303.38	346.3	379.3	404.68	424.46	440.14	452.77
2,3,7,8-TBPZ	185.81	250.05	304.31	347.13	379.99	405.24	424.92	440.52	453.08
penta-BPZ									
1,2,3,4,6-penta-BPZ	202.66	265.65	318.58	360.19	391.95	416.17	434.89	449.59	461.31
1,2,3,4,7-penta-BPZ	203.20	266.41	319.31	360.80	392.44	416.57	435.20	449.83	461.50
1,2,3,6,7-penta-BPZ	202.74	266.13	319.04	360.55	392.22	416.37	435.02	449.67	461.36
1,2,3,6,8-penta-BPZ	203.39	266.62	319.42	360.84	392.43	416.53	435.14	449.75	461.42
1,2,3,6,9-penta-BPZ	202.74	265.84	318.69	360.22	391.94	416.13	434.83	449.51	461.23
1,2,3,7,8-penta-BPZ	203.06	266.71	319.64	361.07	392.65	416.72	435.31	449.90	461.55
1,2,3,7,9-penta-BPZ	203.35	266.61	319.44	360.86	392.45	416.54	435.15	449.77	461.43
1,2,3,8,9-penta-BPZ	202.84	266.22	319.12	360.62	392.27	416.41	435.06	449.71	461.40
1,2,4,6,7-penta-BPZ	202.93	265.85	318.61	360.11	391.82	416.02	434.73	449.42	461.15
1,2,4,6,8-penta-BPZ	203.43	266.25	318.93	360.36	392.00	416.16	434.82	449.48	461.19
1,2,4,6,9-penta-BPZ	202.75	265.40	318.12	359.67	391.44	415.71	434.47	449.20	460.96
1,2,4,7,8-penta-BPZ	203.01	266.28	319.09	360.54	392.18	416.31	434.96	449.60	461.29
1,2,4,7,9-penta-BPZ	203.33	266.13	318.81	360.25	391.91	416.08	434.76	449.43	461.14
1,2,4,8,9-penta-BPZ	202.79	265.75	318.53	360.05	391.77	415.98	434.69	449.39	461.12
hexa-BPZ									
1,2,3,4,6,7-hexa-BPZ	219.88	282.64	334.24	374.38	404.79	427.78	445.36	459.02	469.81
1,2,3,4,6,8-hexa-BPZ	220.44	283.07	334.57	374.64	404.98	427.92	445.46	459.09	469.85
1,2,3,4,6,9-hexa-BPZ	219.74	282.20	333.74	373.93	404.40	427.46	445.10	458.81	469.63
1,2,3,4,7,8-hexa-BPZ	220.10	283.17	334.80	374.87	405.19	428.10	445.62	459.23	469.98
1,2,3,6,7,8-hexa-BPZ	220.15	283.22	334.83	374.89	405.20	428.10	445.62	459.22	469.97
1,2,3,6,7,9-hexa-BPZ	220.12	282.78	334.28	374.36	404.73	427.70	445.27	458.93	469.72
1,2,3,6,8,9-hexa-BPZ	220.06	282.73	334.23	374.31	404.69	427.67	445.24	458.90	469.69
1,2,3,7,8,9-hexa-BPZ	220.09	283.19	334.81	374.87	405.18	428.09	445.60	459.21	469.96
1,2,4,6,7,9-hexa-BPZ	219.88	282.10	333.49	373.62	404.08	427.15	444.80	458.53	469.38
1,2,4,6,8,9-hexa-BPZ	220.11	282.31	333.67	373.77	404.20	427.25	444.89	458.61	469.44
hepta-BPZ									
1,2,3,4,6,7,8-hepta-BPZ	237.33	299.79	350.08	388.77	417.81	439.55	455.98	468.60	478.44
1,2,3,4,6,7,9-hepta-BPZ	237.33	299.34	349.50	388.21	417.31	439.12	455.62	468.29	478.18
OBPZ									
1,2,3,4,6,7,8,9-OBPZ	254.38	316.20	365.18	402.52	430.30	450.89	466.27	477.90	486.85

As a result of the recalculation, eqs 10 through 12 should be replaced by the following:

$$S^{\Theta}/\text{J·mol}^{-1}\text{·K}^{-1} = 395.80 + 41.40N_{\alpha} + 42.67N_{\beta} - 3.25N_{o} \qquad R^2 = 1.000,\ \text{SD} = 3.51 \qquad (10)$$

$$\Delta_f H^{\Theta}/\text{kJ·mol}^{-1} = 342.54 + 30.38N_{\alpha} + 26.03N_{\beta} + 1.21N_{1,9} + 8.99N_{o} + 2.82N_{m} + 1.58N_{p}$$
$$R^2 = 0.9995,\ \text{SD} = 1.29 \qquad (11)$$

$$\Delta_f G^{\theta}/\mathrm{kJ{\cdot}mol^{-1}} = 358.03 + 37.18N_{\alpha} + 30.31N_{\beta} - 4.50N_{1,9} + 3.53N_{o} - 3.68N_{m} - 3.42N_{p}$$
$$R^2 = 0.9110, \mathrm{SD} = 16.32 \qquad (12)$$

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Thermophysical Properties of *N*-Octyl-3-methylpyridinium Tetrafluoroborate. Isabel Bandrés, Beatriz Giner, Héctor Artigas, Carlos Lafuente, and Félix M. Royo,* *J. Chem. Eng. Data* **2009,** *54*, 236–240.

In the ninth column of Table 1 of the original paper (*J. Chem. Eng. Data* **2009**, *54*, 236−240), the isobaric heat capacity values of *n*-octyl-3-methylpyridinium tetrafluoroborate are reported. Because of a calculation error, these data are wrong. The correct data are shown below.

Table 1

T/K	$C_{P,m}$/J·mol^{-1}·K^{-1}
278.15	573
280.65	575
283.15	577
285.65	579
288.15	580
290.65	582
293.15	584
295.65	587
298.15	589
300.65	591
303.15	594
305.65	595
308.15	598
310.65	600
313.15	602
315.65	604
318.15	606
320.65	608
323.15	610
325.65	612
328.15	614

The correlation equation of these isobaric heat capacity data and the corresponding standard deviation are:

$$C_{p,m}/\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}} = 0.8298(T/\mathrm{K}) + 342$$
$$s = 1\ \mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$$

The authors apologize for this mistake.

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