Density Functional Theory Calculation on Polychlorinated Anthraquinones: Their Gas Phase Thermodynamic Function and Implication of the Cl Substituted Position. Chen Wang, Hong X. Liu, Zhe Y. Fang, and Zun Y. Wang,* *J. Chem. Eng. Data* DOI: 10.021/je9003564.

Because the molecular symmetry was missed in the calculation process, the values of je-2009-003564 have been corrected considering molecular symmetry. All molecules were calculated at the B3LYP/6-31G* level, and the vibrational scaling factor is 0.96.

Eq 13 should be replaced by:

$$S^{\theta}/\mathrm{J\cdot mol^{-1}\cdot K^{-1}} = 448.90 + 29.18N$$
$$R^2 = 0.980 \qquad \mathrm{SE} = 6.40 \qquad F = 3657.873 \tag{13}$$

Equations 14 and 15 should be replaced by:

$$\Delta_f H^{\theta}/\mathrm{kJ\cdot mol^{-1}} = -118.218 + 1.424N_{\alpha} - 26.971N_{\beta} + 14.712N_{o} + 3.212N_{m} + 4.173N_{p}$$
$$R^2 = 0.988 \qquad \mathrm{SE} = 2.352 \qquad F = 1139.471 \tag{14}$$

$$\Delta_f G^{\theta}/\mathrm{kJ\cdot mol^{-1}} = -8.886 + 5.733N_{\alpha} - 21.994N_{\beta} + 15.329N_{o} + 3.321N_{m} + 5.549N_{p}$$
$$R^2 = 0.990 \qquad \mathrm{SE} = 2.398 \qquad F = 1352.333 \tag{15}$$

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Table 5. Thermodynamic Parameters of PCAQNs Computed at B3LYP/6-31G* Level and N_{PCS}[a]

			S^θ	$\Delta_f H^\theta$	$\Delta_f G^\theta$	$\Delta_f G^\theta_R$	$C_{p,m}$/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}	R^2	SE	N_α	N_β	N_o	N_m	N_p	$N_{1,8}$
AQN	D_{2h}	4	430.53	−119.40	−6.26		565.63	43.76	−1.60	1.47	1.000	1.34	0	0	0	0	0	0
mono-CAQN																		
1	C_1	1	476.54	−117.93	−4.31	27.56	578.77	36.17	−1.57	1.42	1.000	1.28	1	0	0	0	0	0
2	C_s	1	473.08	−146.53	−31.87	0.00	578.09	36.55	−1.57	1.42	1.000	1.29	0	1	0	0	0	0
di-CAQN																		
1,2	C_1	1	507.44	−129.25	−10.63	40.86	591.84	28.76	−1.54	1.37	1.000	1.23	1	1	1	0	0	0
1,3	C_1	1	507.10	−142.24	−23.52	27.96	591.39	28.93	−1.53	1.37	1.000	1.23	1	1	0	1	0	0
1,4	C_s	1	514.88	−108.29	8.11	59.59	591.78	28.65	−1.53	1.36	1.000	1.23	2	0	0	0	1	0
1,5	C_2	2	517.75	−116.80	−1.26	50.23	591.84	28.65	−1.53	1.36	1.000	1.23	2	0	0	0	0	0
1,6	C_1	1	507.32	−144.56	−25.90	25.58	591.18	29.00	−1.53	1.36	1.000	1.24	1	1	0	0	0	0
1,7	C_1	1	507.20	−144.71	−26.02	25.46	591.28	28.94	−1.53	1.36	1.000	1.23	1	1	0	0	0	0
1,8	C_s	1	505.21	−114.53	4.75	56.24	591.44	28.84	−1.53	1.36	1.000	1.23	2	0	0	0	0	1
2,3	C_{2v}	2	496.03	−160.75	−38.73	12.75	590.48	29.61	−1.53	1.37	1.000	1.25	0	2	1	0	0	0
2,6	C_{2h}	2	497.50	−173.07	−51.49	0.00	590.49	29.39	−1.53	1.36	1.000	1.24	0	2	0	0	0	0
2,7	C_{2v}	2	497.60	−172.94	−51.39	0.10	590.55	29.34	−1.53	1.36	1.000	1.24	0	2	0	0	0	0
tri-CAQN																		
1,2,3	C_1	1	537.04	−140.20	−16.20	45.01	604.81	21.51	−1.51	1.32	1.000	1.19	1	2	2	1	0	0
1,2,4	C_1	1	540.64	−116.93	5.99	67.21	604.71	21.37	−1.50	1.31	1.000	1.18	2	1	1	1	1	0
1,2,5	C_1	1	541.94	−128.05	−5.52	55.70	604.78	21.30	−1.50	1.31	1.000	1.18	2	1	1	0	0	0
1,2,6	C_1	1	537.84	−155.40	−31.64	29.58	604.21	21.63	−1.50	1.31	1.000	1.19	1	2	1	0	0	0
1,2,7	C_1	1	538.48	−155.42	−31.86	29.36	604.39	21.52	−1.50	1.31	1.000	1.19	1	2	1	0	0	0
1,2,8	C_1	1	533.09	−126.27	−1.09	60.13	604.24	21.61	−1.50	1.31	1.000	1.18	2	1	1	0	0	1
1,3,5	C_1	1	544.98	−140.87	−19.24	41.97	604.59	21.35	−1.50	1.31	1.000	1.18	2	1	0	1	0	0
1,3,6	C_1	1	537.80	−168.13	−44.36	16.86	603.94	21.69	−1.50	1.31	1.000	1.19	1	2	0	1	0	0
1,3,7	C_1	1	537.76	−168.42	−44.63	16.59	604.04	21.62	−1.50	1.31	1.000	1.18	1	2	0	1	0	0
1,3,8	C_1	1	535.83	−138.27	−13.92	47.30	604.08	21.62	−1.50	1.31	1.000	1.18	2	1	0	1	0	1
1,4,5	C_1	1	535.25	−109.56	14.97	76.19	604.02	21.58	−1.49	1.30	1.000	1.18	3	0	0	0	1	1
1,4,6	C_1	1	546.90	−134.65	−13.60	47.62	604.33	21.40	−1.50	1.31	1.000	1.18	2	1	0	0	1	0
2,3,5	C_1	1	536.06	−158.39	−34.10	27.12	603.65	22.03	−1.50	1.31	1.000	1.20	1	2	1	0	0	0
2,3,6	C_1	1	532.59	−186.54	−61.22	0.00	603.01	22.39	−1.50	1.31	1.000	1.20	0	3	1	0	0	0
TCAQN																		
1,2,3,4	C_s	1	566.58	−110.07	19.32	84.91	618.85	13.53	−1.47	1.27	1.000	1.13	2	2	3	2	1	0
1,2,3,5	C_1	1	585.04	−138.77	−14.88	50.71	617.96	13.97	−1.47	1.27	1.000	1.14	2	2	2	1	0	0
1,2,3,6	C_1	1	567.06	−165.80	−36.55	29.04	617.37	14.27	−1.47	1.27	1.000	1.15	1	3	2	1	0	0
1,2,3,7	C_1	1	566.65	−166.03	−36.66	28.93	617.33	14.29	−1.47	1.27	1.000	1.14	1	3	2	1	0	0
1,2,3,8	C_1	1	561.96	−136.74	−5.97	59.62	617.23	14.36	−1.47	1.26	1.000	1.14	2	2	2	1	0	1
1,2,4,5	C_1	1	564.33	−118.27	11.80	77.38	616.97	14.32	−1.46	1.26	1.000	1.13	3	1	1	1	1	1
1,2,4,6	C_1	1	572.13	−142.72	−14.98	50.60	617.38	14.08	−1.47	1.26	1.000	1.13	2	2	1	1	1	0
1,2,4,7	C_1	1	572.17	−142.61	−14.88	50.70	617.33	14.10	−1.46	1.26	1.000	1.13	2	2	1	1	1	0
1,2,4,8	C_1	1	564.05	−118.85	11.30	76.88	616.94	14.35	−1.46	1.26	1.000	1.13	3	1	1	1	1	1
1,2,5,6	C_2	2	563.81	−139.00	−8.78	56.80	617.62	14.07	−1.47	1.26	1.000	1.13	2	2	2	0	0	0
1,2,5,7	C_1	1	582.41	−151.51	−26.84	38.74	617.61	13.99	−1.47	1.26	1.000	1.13	2	2	1	1	0	0
1,2,5,8	C_1	1	564.65	−121.28	8.69	74.27	616.67	14.46	−1.46	1.25	1.000	1.13	3	1	1	0	1	1
1,2,6,7	C_1	1	566.88	−168.81	−39.50	26.08	616.84	14.56	−1.47	1.26	1.000	1.15	1	3	2	0	0	0
1,2,6,8	C_1	1	563.75	−149.46	−19.22	46.36	617.02	14.29	−1.46	1.26	1.000	1.14	2	2	1	1	0	1
1,2,7,8	C_s	1	561.89	−137.65	−6.86	58.72	617.10	14.34	−1.47	1.26	1.000	1.14	2	2	2	0	0	1
1,3,5,7	C_2	2	569.82	−164.31	−35.88	29.70	617.24	14.12	−1.47	1.26	1.000	1.13	2	2	0	2	0	0
1,3,5,8	C_1	1	566.85	−132.45	−3.14	62.45	616.64	14.37	−1.46	1.25	1.000	1.13	3	1	0	1	1	1
1,3,6,7	C_1	1	566.30	−181.67	−52.19	13.39	616.35	14.76	−1.46	1.26	1.000	1.15	1	3	1	1	0	0
1,3,6,8	C_s	1	566.85	−161.16	−31.84	33.74	616.70	14.40	−1.46	1.26	1.000	1.14	2	2	0	2	0	1
1,4,5,8	C_{2v}	2	559.11	−107.25	24.38	89.96	616.07	14.66	−1.45	1.25	1.000	1.13	4	0	0	0	2	2
1,4,6,7	C_s	1	579.53	−148.09	−22.56	43.03	616.78	14.46	−1.46	1.26	1.000	1.14	2	2	1	0	1	0
2,3,6,7	D_{2h}	4	549.97	−199.93	−65.58	0.00	615.50	15.40	−1.47	1.26	1.000	1.16	0	4	2	0	0	0
penta-CAQN																		
1,2,3,4,5	C_1	1	591.92	−112.67	23.38	67.52	630.91	6.61	−1.44	1.22	1.000	1.08	3	2	3	2	1	1
1,2,3,4,6	C_1	1	597.28	−135.49	−1.04	43.10	631.45	6.26	−1.44	1.22	1.000	1.08	2	3	3	2	1	0
1,2,3,5,6	C_1	1	601.51	−149.35	−16.17	27.97	630.90	6.65	−1.44	1.22	1.000	1.09	2	3	3	1	0	0
1,2,3,5,7	C_1	1	608.75	−161.89	−30.86	13.28	630.72	6.68	−1.44	1.22	1.000	1.09	2	3	2	2	0	0
1,2,3,5,8	C_1	1	592.81	−131.48	4.30	48.44	629.79	7.13	−1.43	1.21	1.000	1.09	3	2	2	1	1	1
1,2,3,6,7	C_1	1	595.68	−179.06	−44.14	0.00	629.89	7.28	−1.44	1.22	1.000	1.10	1	4	3	1	0	0
1,2,3,6,8	C_1	1	592.97	−159.32	−23.58	20.56	629.93	7.11	−1.43	1.22	1.000	1.09	2	3	2	2	0	1
1,2,3,7,8	C_1	1	590.29	−147.84	−11.31	32.83	630.13	7.07	−1.44	1.22	1.000	1.10	2	3	3	1	0	1
1,2,4,5,6	C_1	1	593.86	−129.78	5.68	49.82	629.80	7.08	−1.43	1.21	1.000	1.09	3	2	2	1	1	1
1,2,4,5,7	C_1	1	595.15	−140.92	−5.84	38.31	629.56	7.14	−1.43	1.21	1.000	1.08	3	2	1	2	1	1
1,2,4,5,8	C_1	1	593.45	−116.78	18.81	62.95	629.01	7.40	−1.42	1.20	1.000	1.08	4	1	1	1	2	2
1,2,4,6,7	C_1	1	601.87	−155.72	−22.64	21.50	629.91	7.08	−1.43	1.21	1.000	1.09	2	3	2	1	1	0
1,2,4,6,8	C_1	1	594.94	−141.49	−6.35	37.79	629.62	7.09	−1.43	1.21	1.000	1.08	3	2	1	2	1	1
1,2,4,7,8	C_1	1	592.84	−130.54	5.22	49.36	629.76	7.12	−1.43	1.21	1.000	1.09	3	2	2	1	1	1
hexa-CAQN																		
1,2,3,4,5,6	C_1	1	620.53	−124.24	17.49	36.37	643.74	−0.62	−1.40	1.17	1.000	1.04	3	3	4	2	1	1
1,2,3,4,5,7	C_1	1	622.80	−134.93	6.11	24.99	643.63	−0.66	−1.40	1.17	1.000	1.03	3	3	3	3	1	1
1,2,3,4,5,8	C_s	1	620.63	−111.57	30.12	49.00	642.87	−0.25	−1.40	1.16	1.000	1.04	4	2	3	2	2	2

Table 5. Continued

			S^θ	$\Delta_f H^\theta$	$\Delta_f G^\theta$	$\Delta_f G^\theta_R$	$C_{p,m}$/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}	R^2	SE	N_α	N_β	N_o	N_m	N_p	$N_{1,8}$
1,2,3,4,6,7	C_s	1	627.52	−148.21	−8.58	10.31	644.00	−0.74	−1.41	1.17	1.000	1.04	2	4	4	2	1	0
1,2,3,5,6,7	C_2	2	624.17	−159.52	−18.88	0.00	643.99	−0.65	−1.41	1.17	1.000	1.05	2	4	4	2	0	0
1,2,3,5,6,8	C_1	1	622.19	−139.63	1.60	20.48	642.86	−0.21	−1.40	1.16	1.000	1.04	3	3	3	2	1	1
1,2,3,5,7,8	C_1	1	622.22	−140.16	1.06	19.94	642.85	−0.19	−1.40	1.16	1.000	1.05	3	3	3	2	1	1
1,2,3,6,7,8	C_s	1	619.63	−157.45	−15.46	3.42	643.16	−0.20	−1.41	1.17	1.000	1.05	2	4	4	2	0	1
1,2,4,5,6,8	C_2	2	616.80	−125.79	17.04	35.92	641.99	0.13	−1.39	1.16	1.000	1.04	4	2	2	2	2	2
1,2,4,5,7,8	C_s	1	622.60	−125.79	15.32	34.20	641.89	0.20	−1.39	1.16	1.000	1.04	4	2	2	2	2	2
hepta-CAQN																		
1,2,3,4,5,6,7	C_1	1	649.21	−133.77	13.60	0.00	656.70	−7.84	−1.37	1.12	1.000	1.00	3	4	5	3	1	1
1,2,3,4,5,6,8	C_1	1	649.05	−120.75	26.67	13.07	655.71	−7.43	−1.37	1.11	1.000	1.00	4	3	4	3	2	2
OCAQN																		
1,2,3,4,5,6,7,8	C_{2v}	2	670.78	−115.44	39.71		669.53	−15.07	−1.34	1.07	1.000	0.95	4	4	6	4	2	2

[a] V_m is the molecular volume. 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. $\Delta_f G^\theta_R$ is the relative magnitude of the standard Gibbs energy of formation. $C^\theta_{p,m}$ is the molar heat capacity at constant pressure. N is the number of Cl atom substitutions, and the subscript PCS indicates the positions.

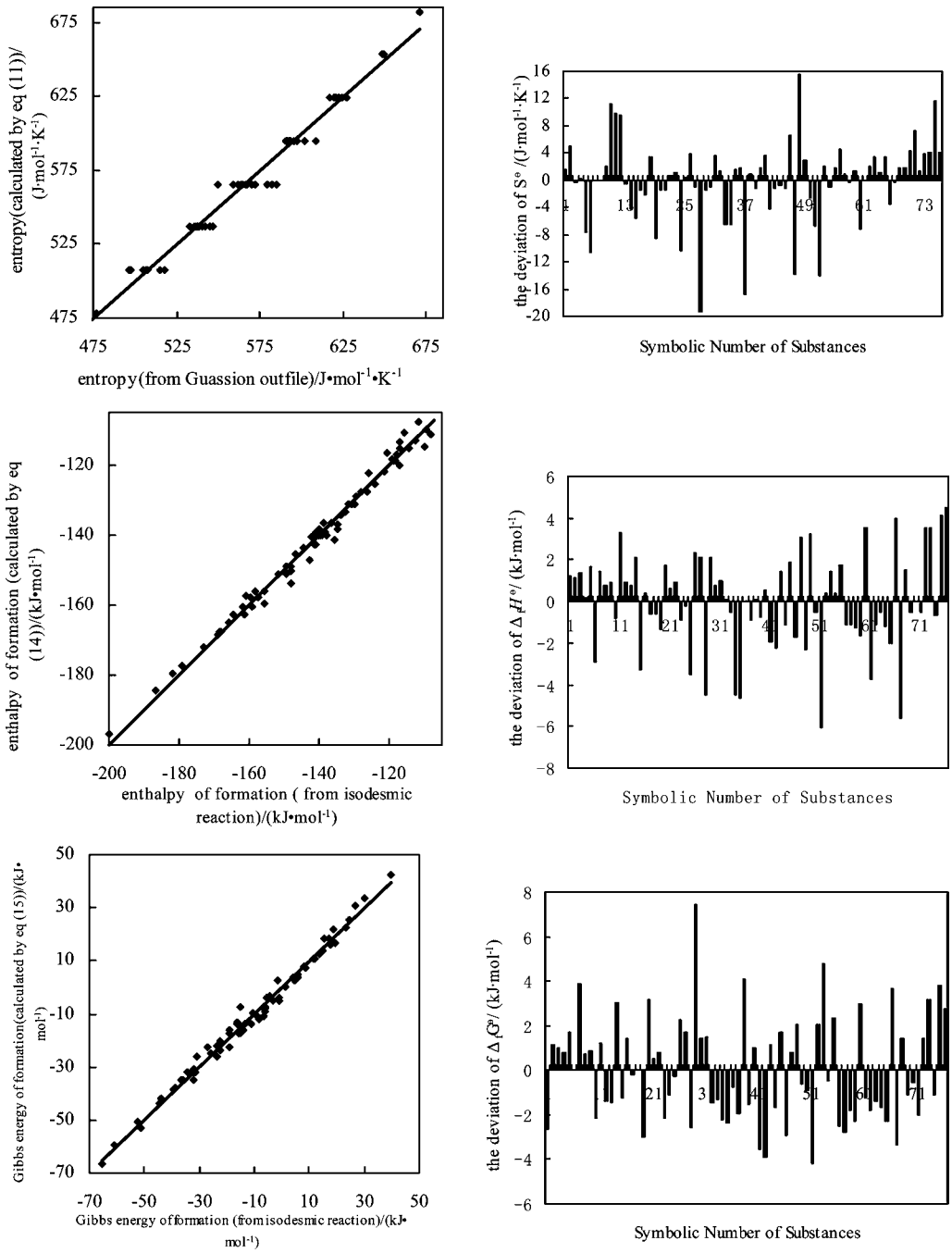

Figure 2. Plots of the values obtained from the correlations versus the corresponding DFT results.