Table 1. Calculated theoretical chemical parameters for OPD and PPD additives

Descriptor	OPD (aqueous)	PPD (aqueous)	OPD (gas)	PPD (gas)
HOMO	-5.522	-5.361	-5.037	-4.955
LUMO	-2.936	-3.159	-2.459	-2.77
ΔE(HOMO-LUMO)	-2.586	-2.202	2.578	2.185
Ionization energy (I)	4.716	4.785	5.037	4.955
Electron affinity A)	1.9178	2.066	2.459	2.77
Dipole moment (Debye)	4.390	5.982	2.5561	3.6915
Electronegativity (X)	3.347	3.426	3.748	3.8625
Global hardness (η)	1.369	1.360	1.289	1.0925
Chemical potential (π)	-3.347	-3.426	-3.748	-3.8625
Global softness (σ)	0.730	0.736	0.7758	0.9153
Global electrophilicity (ω)	4.091	4.316	5.449	6.8279
Electrodonating (ω-) power	5.936	6.198	7.4841	8.8957
Electroaccepting (ω+) power	2.589	2.773	3.7361	5.0332
Net electrophilicity (Δω+-)	2.421	2.611	3.6025	4.9208
Polarizability (a.u)	572.971	650.707		

Table 2. Fukui radical, negative and positive indices values for the OPD additive

	Radial attack		Nucleophilic Attack (Fukui(+))		Electrophilic Attack (Fukui(−))	
atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld
C (1)	0.014	0.019	0.007	0.013	0.02	0.024
C (2)	0.018	0.019	0.017	0.017	0.018	0.022
C (3)	-0.001	0.01	-0.006	0.01	0.003	0.01
C (4)	0.012	0.012	0.018	0.015	0.005	0.009
C (5)	0.014	0.018	0.005	0.011	0.022	0.024
C (6)	0.015	0.02	0.02	0.023	0.011	0.017
C (7)	0.043	0.041	0.057	0.051	0.03	0.031
C (8)	0.011	0.018	0.013	0.023	0.009	0.013
C (9)	0.03	0.03	0.035	0.033	0.025	0.027
C (10)	0.016	0.025	0.004	0.017	0.027	0.033
C (11)	0.039	0.038	0.061	0.056	0.018	0.021
N (12)	0.023	0.032	0.021	0.033	0.026	0.031
C (13)	0.024	0.025	0.019	0.018	0.029	0.033
C (14)	0.024	0.026	0.019	0.018	0.029	0.033
C (15)	0.011	0.018	0.008	0.015	0.013	0.02
C (16)	0.025	0.031	0.019	0.023	0.031	0.038
C (17)	0.025	0.03	0.019	0.023	0.031	0.038
C (18)	0.011	0.018	0.008	0.016	0.013	0.02
N (19)	0.023	0.032	0.02	0.032	0.026	0.031
C (20)	0.039	0.038	0.06	0.055	0.018	0.021
C (21)	0.016	0.025	0.004	0.017	0.028	0.034
C (22)	0.03	0.03	0.034	0.032	0.026	0.027
C (23)	0.011	0.018	0.013	0.023	0.009	0.013
C (24)	0.043	0.04	0.055	0.05	0.03	0.031
C (25)	-0.001	0.01	-0.006	0.01	0.003	0.01
C (26)	0.012	0.012	0.018	0.015	0.006	0.009
C (27)	0.017	0.019	0.017	0.017	0.018	0.022
C (28)	0.014	0.019	0.007	0.013	0.02	0.024
C (29)	0.015	0.019	0.019	0.022	0.011	0.017
C (30)	0.014	0.018	0.005	0.011	0.023	0.025
O (31)	0.028	0.028	0.025	0.027	0.031	0.029
O (32)	0.028	0.028	0.024	0.026	0.031	0.029
H (33)	0.014	0.009	0.012	0.008	0.016	0.011
H (34)	0.016	0.01	0.015	0.009	0.016	0.01
H (35)	0.014	0.009	0.012	0.007	0.016	0.01
H (36)	0.014	0.01	0.014	0.01	0.014	0.009
H (37)	0.023	0.017	0.027	0.02	0.019	0.013
H (38)	0.019	0.012	0.022	0.014	0.016	0.01
H (39)	0.028	0.016	0.032	0.019	0.025	0.013
H (40)	0.02	0.012	0.018	0.011	0.022	0.013

H (41)	0.021	0.014	0.017	0.012	0.025	0.017
H (42)	0.021	0.014	0.017	0.012	0.025	0.017
H (43)	0.02	0.012	0.018	0.011	0.022	0.013
H (44)	0.028	0.016	0.032	0.019	0.025	0.013
H (45)	0.019	0.012	0.022	0.014	0.016	0.01
H (46)	0.023	0.016	0.026	0.02	0.019	0.013
H (47)	0.015	0.01	0.014	0.009	0.016	0.01
H (48)	0.014	0.009	0.012	0.008	0.016	0.011
H (49)	0.014	0.01	0.014	0.01	0.014	0.009
H (50)	0.014	0.009	0.012	0.007	0.016	0.01
H (51)	0.012	0.009	0.012	0.009	0.011	0.01
H (52)	0.012	0.009	0.012	0.009	0.011	0.01

Table 3. Fukui radical, negative and positive indices values for the PPD additive

	Radical Attack (Fukui(0))		Nucleophilic Attack (Fukui(+))		Electrophilic Attack (Fukui(-))	
atom	Mulliken	Hirshfeld	Mulliken	Hirshfeld	Mulliken	Hirshfeld
C (1)	0.026	0.032	0.023	0.028	0.029	0.036
C (2)	0.022	0.027	0.02	0.026	0.024	0.028
C (3)	0.022	0.027	0.02	0.026	0.024	0.028
C (4)	0.026	0.032	0.023	0.028	0.029	0.037
C (5)	0.02	0.024	0.018	0.02	0.022	0.027
C (6)	0.02	0.024	0.018	0.02	0.022	0.027
N (7)	0.018	0.03	0.015	0.031	0.021	0.03
N (8)	0.018	0.03	0.015	0.031	0.021	0.03
C (9)	0.051	0.045	0.077	0.066	0.025	0.025
C (10)	0.051	0.045	0.077	0.066	0.025	0.025
C (11)	0.012	0.024	-0.003	0.014	0.026	0.034
C (12)	0.012	0.024	-0.003	0.014	0.026	0.034
C (13)	0.012	0.012	0.019	0.014	0.006	0.009
C (14)	-0.001	0.01	-0.005	0.009	0.003	0.01
C (15)	0.041	0.039	0.05	0.046	0.032	0.033
C (16)	0.009	0.016	0.009	0.019	0.008	0.013
C (17)	0.031	0.031	0.035	0.032	0.028	0.029
C (18)	0.031	0.031	0.034	0.032	0.028	0.029
C (19)	0.008	0.016	0.009	0.019	0.008	0.013
C (20)	0.041	0.039	0.05	0.045	0.032	0.033
C (21)	-0.001	0.009	-0.005	0.009	0.003	0.01
C (22)	0.012	0.011	0.019	0.014	0.006	0.009
C (23)	0.012	0.016	0.003	0.008	0.021	0.023
C (24)	0.014	0.018	0.016	0.019	0.011	0.017
C (25)	0.013	0.017	0.007	0.012	0.019	0.023
C (26)	0.015	0.017	0.013	0.014	0.017	0.02
C (27)	0.015	0.017	0.013	0.014	0.017	0.02
C (28)	0.013	0.017	0.007	0.012	0.019	0.023
C (29)	0.014	0.018	0.016	0.019	0.011	0.017
C (30)	0.012	0.016	0.003	0.008	0.021	0.023
O (31)	0.029	0.029	0.026	0.027	0.032	0.03
O (32)	0.029	0.029	0.026	0.027	0.032	0.03
H	0.023	0.014	0.022	0.014	0.024	0.015

(33)						
H (34)	0.023	0.014	0.022	0.014	0.024	0.015
H (35)	0.021	0.013	0.019	0.012	0.023	0.014
H (36)	0.021	0.013	0.019	0.012	0.023	0.014
H (37)	0.026	0.016	0.032	0.021	0.021	0.011
H (38)	0.026	0.016	0.032	0.021	0.021	0.011
H (39)	0.022	0.016	0.024	0.018	0.02	0.014
H (40)	0.018	0.011	0.02	0.012	0.017	0.01
H (41)	0.018	0.011	0.02	0.012	0.017	0.01
H (42)	0.022	0.016	0.024	0.018	0.02	0.014
H (43)	0.013	0.008	0.011	0.006	0.015	0.01
H (44)	0.013	0.009	0.012	0.009	0.014	0.009
H (45)	0.013	0.009	0.011	0.007	0.015	0.01
H (46)	0.014	0.009	0.013	0.008	0.016	0.01
H (47)	0.014	0.009	0.013	0.008	0.016	0.01
H (48)	0.013	0.009	0.011	0.007	0.015	0.01
H (49)	0.013	0.009	0.012	0.009	0.014	0.009
H (50)	0.013	0.008	0.011	0.006	0.015	0.01
H (51)	0.012	0.01	0.013	0.009	0.012	0.01
H (52)	0.012	0.01	0.013	0.009	0.012	0.01

Table 4. Respective energetic outputs computed from MD and MC simulations

Parameter	OPD	PPD
Adsorption energy	-121.25 kcal/mol	-195.55 kcal/mol
Interaction energy	-1074.386 kcal/mol	-1132.241 kcal/mol
Binding energy	1074.386 kJ/mol	1132.241 kJ/mol