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Supporting Information for

Application of DFT-based Machine Learning for Developing Molecular Electrode Materials in Li-Ion Battery

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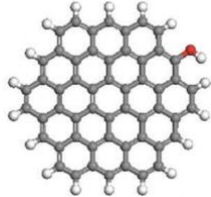
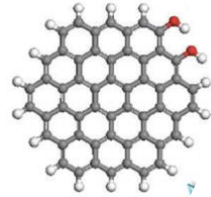
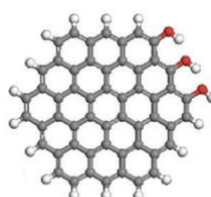
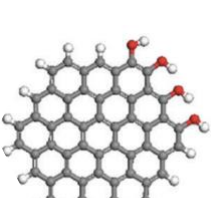
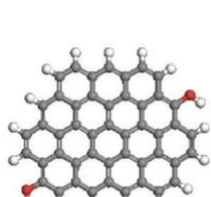
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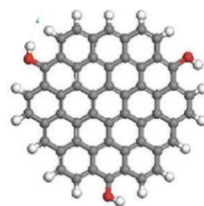
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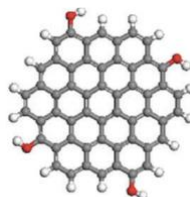
Table S1. Illustrations of graphene functionalized with hydroxyl/carbonyl uniformly or locally distributed. The gray, white, and red colors depict carbon, hydrogen, and oxygen, respectively.

Structure	Illustration
1 Hydroxyl group	
2 Locally distributed hydroxyl groups	
3 Locally distributed hydroxyl groups	
4 Locally distributed hydroxyl groups	
2 uniformly distributed hydroxyl groups	

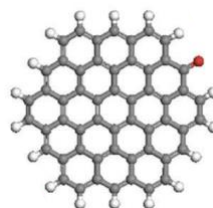
3 uniformly distributed hydroxyl groups



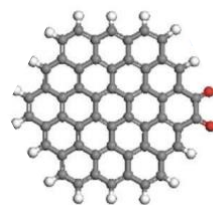
4 uniformly distributed hydroxyl groups



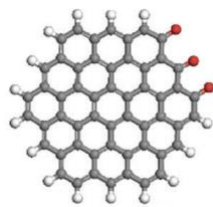
1 Carbonyl group



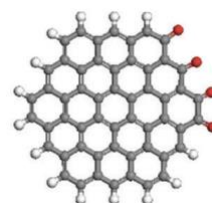
2 Locally distributed carbonyl groups



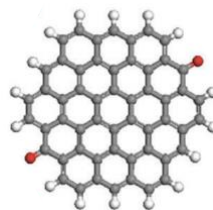
3 Locally distributed carbonyl groups



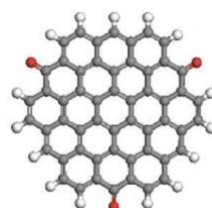
4 Locally distributed carbonyl groups



**2 uniformly
distributed carbonyl
groups**



**3 uniformly
distributed carbonyl
groups**



**4 uniformly
distributed carbonyl
groups**

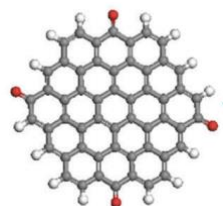
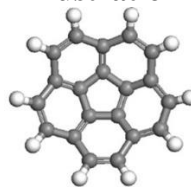


Table S2. Illustrations of chemical structures of the boron-doped corannulene (BDC) molecules as well as pristine corannulene. ‘n’ represents the number of boron atoms and ‘m’ is the case number BDCn-m. The gray, white, and pink colors depict carbon, hydrogen, and boron, respectively.

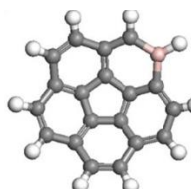
Structure

Illustration

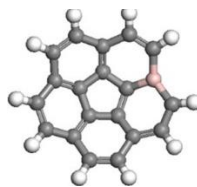
Pristine corannulene



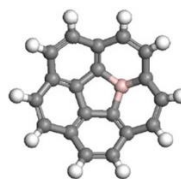
BDC1-1



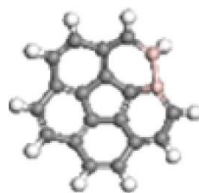
BDC1-2



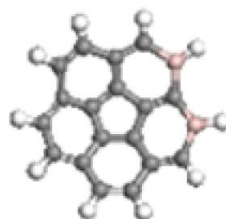
BDC1-3



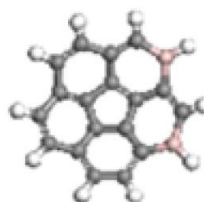
BDC2-1



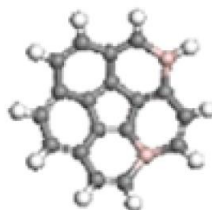
BDC2-2



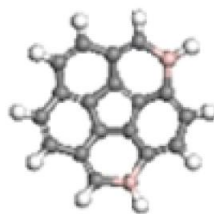
BDC2-3



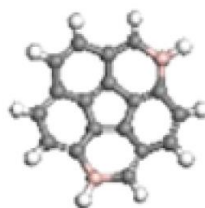
BDC2-4



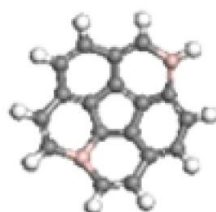
BDC2-5



BDC2-6



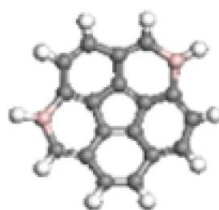
BDC2-7



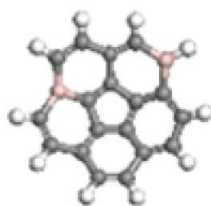
BDC2-8



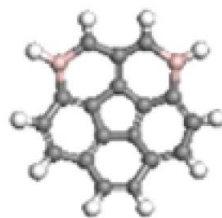
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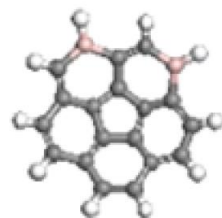
BDC2-10



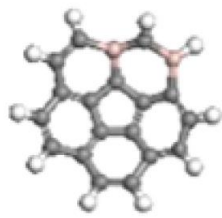
BDC2-11



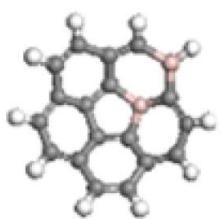
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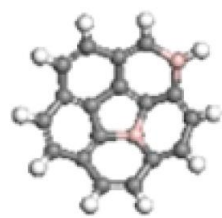
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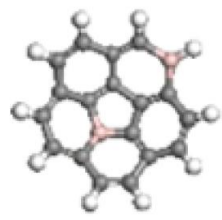
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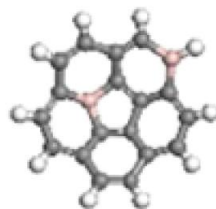
BDC2-16



BDC2-17



BDC2-18



BDC2-19



BDC2-21



BDC2-22



BDC2-23



BDC2-24



BDC2-25



BDC2-26

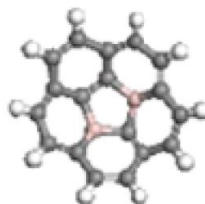
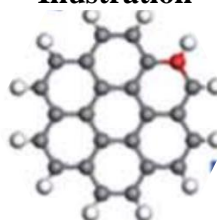


Table S3. Illustrations of one and two-boron doped coronenes are various locations. ‘m’ and ‘n’ in ‘Bm-n’ denote the number of boron dopants and the case number, respectively. The atoms in gray, white, and red are those of carbon, hydrogen, and boron, respectively.

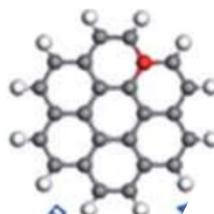
Structure

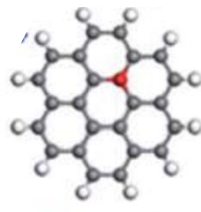
Illustration

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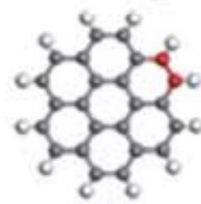


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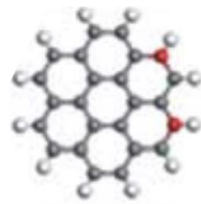




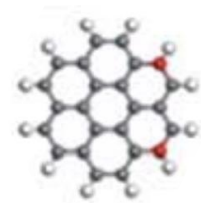
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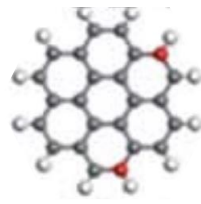
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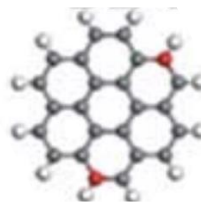
B2-2



B2-3

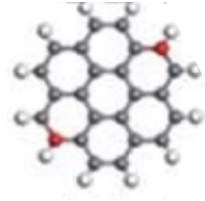


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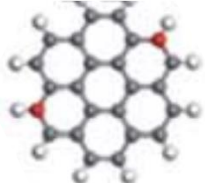


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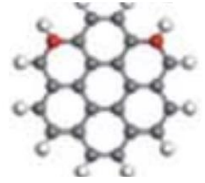
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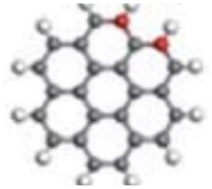
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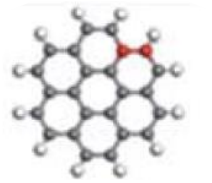
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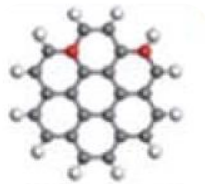
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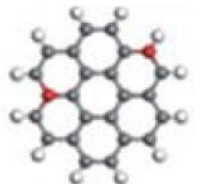
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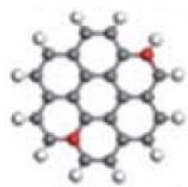
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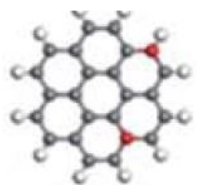
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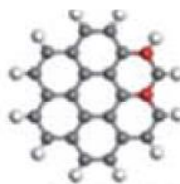
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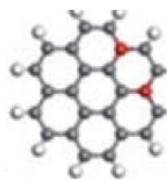
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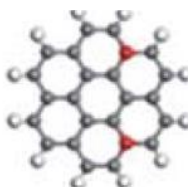
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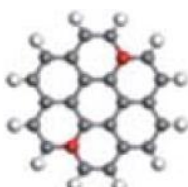
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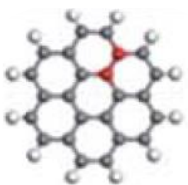
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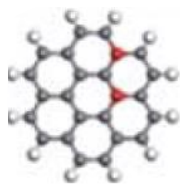
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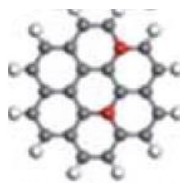
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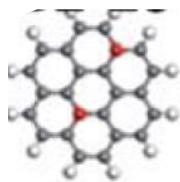
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B2-21



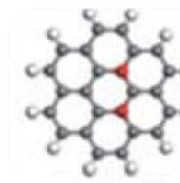
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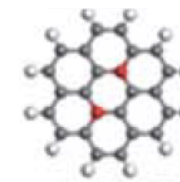
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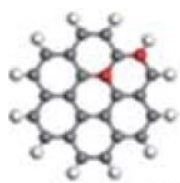
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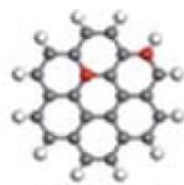
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B2-26



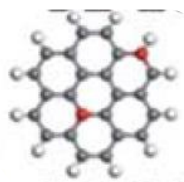
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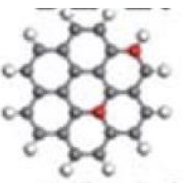
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B2-29



B2-30



B2-31

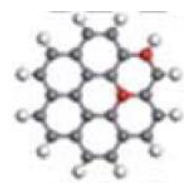
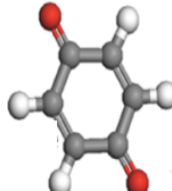
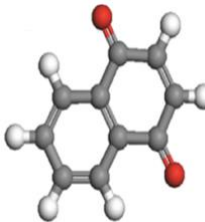
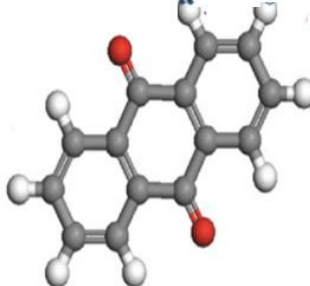
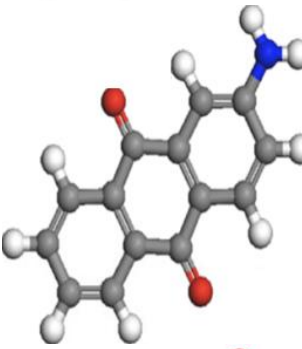
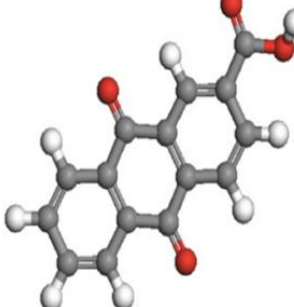
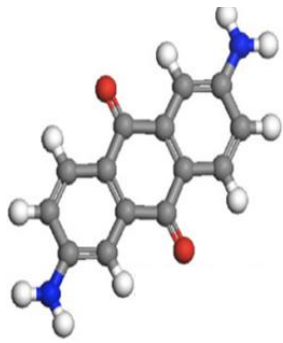


Table S4. Illustrations of the chemical structures of seven quinone derivatives. The atoms in gray, white, red, and blue are those of carbon, hydrogen, oxygen, and nitrogen, respectively.

Structure	Illustration
1,4-Benzoquinone	
1,4-Naphthoquinone	
9,10-Anthraquinone	
2-Aminoanthraquinone	
Anthraquinone-2-carboxylic acid	

**2,6-
Diaminoanthraquinone**



**Anthraquinone-2,6-
dicarboxylic acid**

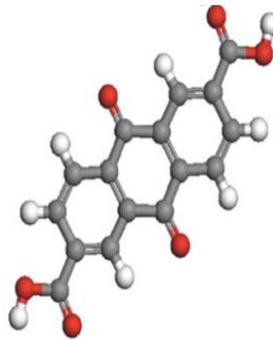

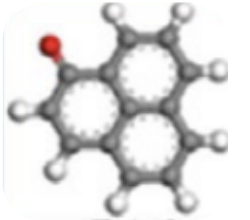
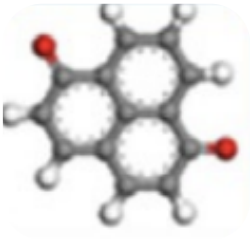
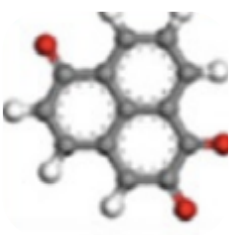
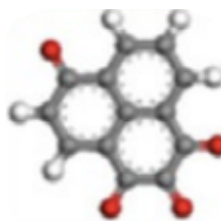


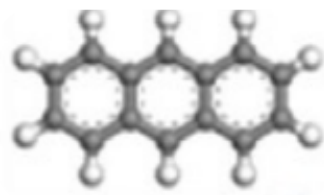
Table S5. Illustrations of ketone derivatives. Up to four carbonyl functional groups were systematically added onto phenalenyl (P) and anthracene (A). ‘a’ and ‘b’ in “Pa-b” and “Aa-b” indicates the number of carbonyl groups and the case number, respectively. The atoms in gray, white, and red are those of carbon, hydrogen, and oxygen, respectively.

Structure	Illustration
P	
P1-2	
P2-4	
P3-3	

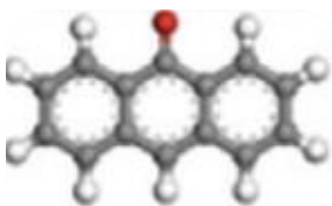
P4-4



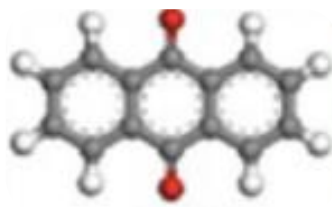
A



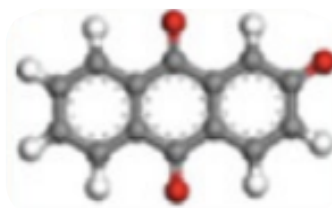
A1-3



A2-5



A3-2



A4-2

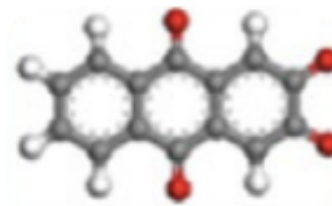


Table S6. Dataset for the DFT and ANN obtained redox potentials (RP) (in V), highest occupied molecular orbital (HOMO) (in eV), lowest unoccupied molecular orbital (LUMO) (in eV), electron affinity (EA) (in eV), and the HOMO-LUMO gap (H-L gap) (in eV) for a variety of organic electrode materials. The redox potentials of highlighted structures were verified experimentally in our previous studies and are in good agreement with the computed values (all fall within ~0.3 V). The DFT RP for A2-5 ketone highlighted in red was erroneously included as 2.20 eV in opposed to 2.30 eV (the actual computed value). As shown, the ANN RP predicted a more accurate RP of 2.28 eV despite being fed erroneous information for that case.

STRUCTURE	RP - DFT	RP - ANN	HOMO	LUMO	EA	H-L GAP
PRISTINE GRAPHENE	1.40	1.89	-5.38	-2.31	-1.52	3.07
1 CARBONYL GROUP	2.90	2.90	-5.02	-2.44	-2.97	2.58
2 LOCALLY DISTRIBUTED CARBONYL GROUPS	3.10	3.12	-5.38	-4.04	-3.29	1.34
3 LOCALLY DISTRIBUTED CARBONYL GROUPS	3.70	3.63	-5.51	-4.25	-3.16	1.26
4 LOCALLY DISTRIBUTED CARBONYL GROUPS	3.60	3.63	-5.80	-4.51	-3.75	1.29
2 UNIFORMLY DISTRIBUTED CARBONYL GROUPS	2.80	2.80	-5.63	-3.81	-3.00	1.82
3 UNIFORMLY DISTRIBUTED CARBONYL GROUPS	3.10	3.14	-5.28	-4.54	-3.41	0.74
4 UNIFORMLY DISTRIBUTED CARBONYL GROUPS	3.20	3.17	-5.51	-5.03	-3.47	0.48
1 HYDROXYL GROUP	1.40	1.48	-5.24	-2.31	-1.53	2.93
2 LOCALLY DISTRIBUTED HYDROXYL GROUPS	1.40	1.44	-5.19	-2.35	-1.61	2.84
3 LOCALLY DISTRIBUTED HYDROXYL GROUPS	1.40	1.33	-5.10	-2.33	-1.55	2.77
4 LOCALLY DISTRIBUTED HYDROXYL GROUPS	1.20	1.20	-5.04	-2.30	-1.38	2.74
2 UNIFORMLY DISTRIBUTED HYDROXYL GROUPS	1.40	1.32	-5.11	-2.32	-1.55	2.79
3 UNIFORMLY DISTRIBUTED HYDROXYL GROUPS	1.30	1.42	-5.17	-2.24	-1.51	2.93
4 UNIFORMLY DISTRIBUTED HYDROXYL GROUPS	1.40	1.40	-5.10	-2.32	-1.58	2.78
PRISTINE CORANNULENE	0.90	0.90	-6.50	-1.81	-0.65	4.69
BDC1-1	3.03	2.98	-6.27	-1.87	-2.67	4.40
BDC1-2	3.32	3.25	-6.22	-1.72	-3.03	4.50
BDC1-3	2.90	2.96	-5.75	-1.78	-2.65	3.97
BDC2-1	2.77	2.79	-6.08	-3.23	-2.54	2.85
BDC2-2	3.09	3.07	-6.25	-1.91	-2.79	4.34
BDC2-3	3.07	3.03	-6.10	-3.99	-2.83	2.11
BDC2-4	3.41	3.33	-6.30	-1.77	-3.16	4.53
BDC2-5	2.96	3.06	-6.30	-1.80	-2.78	4.50
BDC2-6	3.16	3.18	-6.31	-1.90	-2.95	4.41
BDC2-7	3.35	3.33	-6.21	-1.66	-3.15	4.55
BDC2-8	3.00	3.03	-6.35	-3.94	-2.80	2.41
BDC2-9	3.16	3.19	-6.32	-1.90	-2.96	4.42

BDC2-10	2.95	2.99	-6.47	-3.89	-2.74	2.58
BDC2-11	3.01	3.07	-6.34	-1.85	-2.79	4.49
BDC2-12	3.1	3.05	-6.10	-3.99	-2.85	2.11
BDC2-13	3.18	3.16	-6.20	-3.80	-2.93	2.40
BDC2-14	2.51	2.45	-6.67	-3.33	-2.17	3.34
BDC2-15	3.08	3.12	-5.74	-3.95	-2.90	1.79
BDC2-16	3.00	2.99	-5.92	-3.90	-2.79	2.02
BDC2-17	2.97	3.01	-6.03	-3.86	-2.80	2.17
BDC2-18	3.10	3.13	-5.92	-1.84	-2.87	4.08
BDC2-19	2.41	2.46	-6.39	-3.40	-2.19	2.99
BDC2-21	2.92	2.92	-6.45	-3.85	-2.67	2.60
BDC2-22	3.14	3.16	-6.13	-4.21	-2.98	1.92
BDC2-23	2.56	2.57	-6.07	-3.53	-2.34	2.54
BDC2-24	3.08	3.05	-5.67	-3.89	-2.82	1.78
BDC2-25	2.93	2.95	-6.04	-3.85	-2.74	2.19
BDC2-26	2.58	2.59	-6.01	-3.46	-2.35	2.55
BDC2-27	2.50	2.64	-6.07	-3.56	-2.41	2.51
1BORON_1_POSITION1	0.90	0.82	-0.13	-0.06	-0.77	0.07
1BORON_1_POSITION2	0.80	0.88	-0.13	-0.06	-0.85	0.07
1BORON_1_POSITION3	1.10	1.50	-0.13	-0.05	-1.51	0.07
2BORON_1_14_POSITION1	2.20	2.16	-0.14	-0.06	-2.07	0.08
2BORON_1_14_POSITION2	1.90	1.66	-0.14	-0.06	-1.65	0.08
2BORON_1_14_POSITION3	2.10	2.16	-0.14	-0.06	-2.07	0.08
B1-1	5.42	5.39	-5.56	-3.68	-5.17	1.88
B1-2	5.30	5.31	-5.50	-3.72	-5.08	1.78
B1-3	5.28	5.29	-5.62	-3.78	-5.03	1.85
B2-1	2.61	2.54	-5.93	-3.35	-2.29	2.57
B2-2	2.92	2.91	-5.83	-3.75	-2.68	2.07
B2-3	3.57	3.62	-5.34	-4.31	-3.38	1.03
B2-4	3.06	3.08	-6.14	-2.84	-2.85	3.30
B2-5	-0.39	-0.38	-6.21	-3.74	0.66	2.47
B2-6	0.42	0.44	-6.13	-3.95	-0.25	2.18
B2-7	0.46	0.46	-5.43	-4.48	-0.22	0.95
B2-8	0.38	0.43	-5.71	-3.97	-0.17	1.75
B2-9	1.45	1.53	-5.99	-4.07	-1.36	1.92
B2-10	3.00	2.99	-5.66	-3.81	-2.75	1.85
B2-11	3.28	3.33	-5.61	-4.23	-3.13	1.38
B2-12	2.95	2.99	-5.98	-3.89	-2.78	2.10
B2-13	3.07	3.12	-6.23	-2.81	-2.90	3.42
B2-14	2.79	2.80	-6.04	-3.67	-2.58	2.37
B2-15	3.13	3.13	-5.68	-3.98	-2.91	1.70
B2-16	0.50	0.48	-5.86	-3.65	-0.20	2.21
B2-17	1.82	1.83	-5.22	-4.65	-1.57	0.57
B2-18	0.40	0.38	-6.13	-3.82	-0.17	2.31
B2-19	1.93	1.85	-6.08	-3.54	-1.62	2.53
B2-20	3.33	3.34	-5.60	-4.11	-3.11	1.48
B2-21	3.10	3.06	-5.90	-3.98	-2.87	1.91
B2-22	1.12	1.09	-5.80	-4.22	-0.89	1.58
B2-23	3.81	3.76	-5.07	-4.47	-3.51	0.59
B2-24	4.35	4.34	-5.66	-4.20	-4.08	1.46
B2-25	1.37	1.32	-5.59	-4.24	-1.08	1.35
B2-26	3.13	3.09	-6.04	-2.86	-2.86	3.18
B2-27	3.16	3.13	-5.98	-4.01	-2.93	1.98

B2-28	3.14	3.16	-5.95	-2.89	-2.93	3.06
B2-29	3.18	3.19	-5.76	-4.05	-2.99	1.71
B2-30	3.25	3.24	-5.82	-4.11	-3.05	1.71
B2-31	2.70	2.68	-6.05	-3.52	-2.45	2.54
1,4-BENZOQUINONE	2.90	2.90	-8.03	-3.76	-2.17	4.27
1,4-NAPHTHOQUINONE	2.60	2.59	-7.82	-3.39	-2.03	4.43
9,10-ANTHRAQUINONE	2.30	2.28	-7.63	-3.02	-1.77	4.61
2-AMINOANTHRAQUINONE	2.10	2.11	-6.42	-2.72	-1.51	3.70
ANTHRAQUINONE-2-CARBOXYLIC ACID	2.40	2.40				
			-7.82	-3.28	-2.10	4.54
2,6-DIAMINOANTHRAQUINONE	1.90	1.82	-6.10	-2.40	-1.25	3.70
ANTHRAQUINONE-2,6-DICARBOXYLIC ACID WITH 1LI	1.79	2.63				
			-5.77	-2.42	-1.63	3.34
1,4-BENZOQUINONE WITH 2LI	-1.24	-1.78	-3.47	-1.04	-0.74	2.43
1,4-NAPHTHOQUINONE WITH 2LI	-1.80	-1.81	-3.45	-1.13	-0.82	2.32
9,10-ANTHRAQUINONE WITH 2LI	-1.63	-1.89	-3.34	-1.24	-0.91	2.10
2,6-DIAMINOANTHRAQUINONE WITH 2LI	-1.74	-2.11				
			-2.86	-1.14	-0.83	1.71
ANTHRAQUINONE-2,6-DICARBOXYLIC ACID WITH 2LI	0.47	0.31				
			-3.93	-1.57	-1.20	2.36
P	1.85	1.85	-4.63	-0.44	-1.38	4.19
P1-2	1.87	1.87	-6.55	-2.72	-1.39	3.83
P2-4	3.48	3.41	-6.44	-2.59	-3.13	3.85
P3-3	3.12	3.54	-7.59	-4.04	-2.79	3.55
P4-4	3.93	3.93	-7.20	-3.91	-3.78	3.29
A	0.95	0.94	-5.66	-1.83	-0.56	3.84
A1-3	2.68	2.61	-5.57	-1.67	-2.23	3.90
A3-2	3.82	3.81	-7.22	-3.25	-3.42	3.96
A4-2	3.51	3.71	-7.77	-4.48	-3.14	3.29