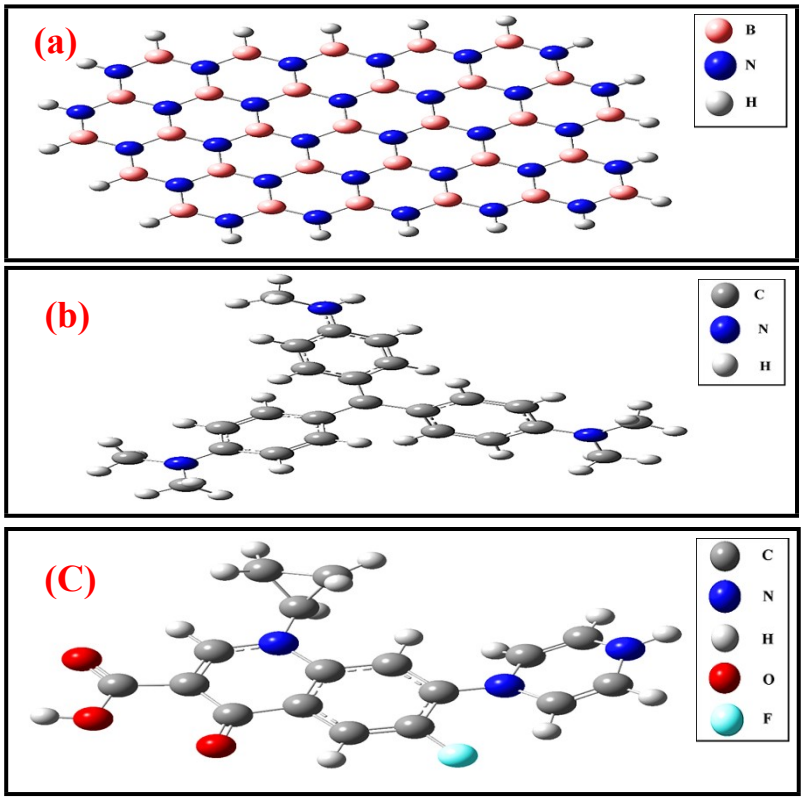
Supplementary Information (SI)

Simultaneous adsorption of ciprofloxacin drug and methyl violet dye on boron nitride nanosheets: experimental and theoretical insights

Keivan Javanmard, Saeed Farhadi,* and Abedin Zabardasti,*

Department of Inorganic Chemistry, Faculty of Chemistry, Lorestan University, Khorramabad, 68151-44316, Iran
*Corresponding authors: Tel: +986633120611, fax: +986633120618.
Email addresses: farhadi.s@lu.ac.ir (S. Farhadi), zabardasti.a@lu.ac.ir (A. Zabardasti)



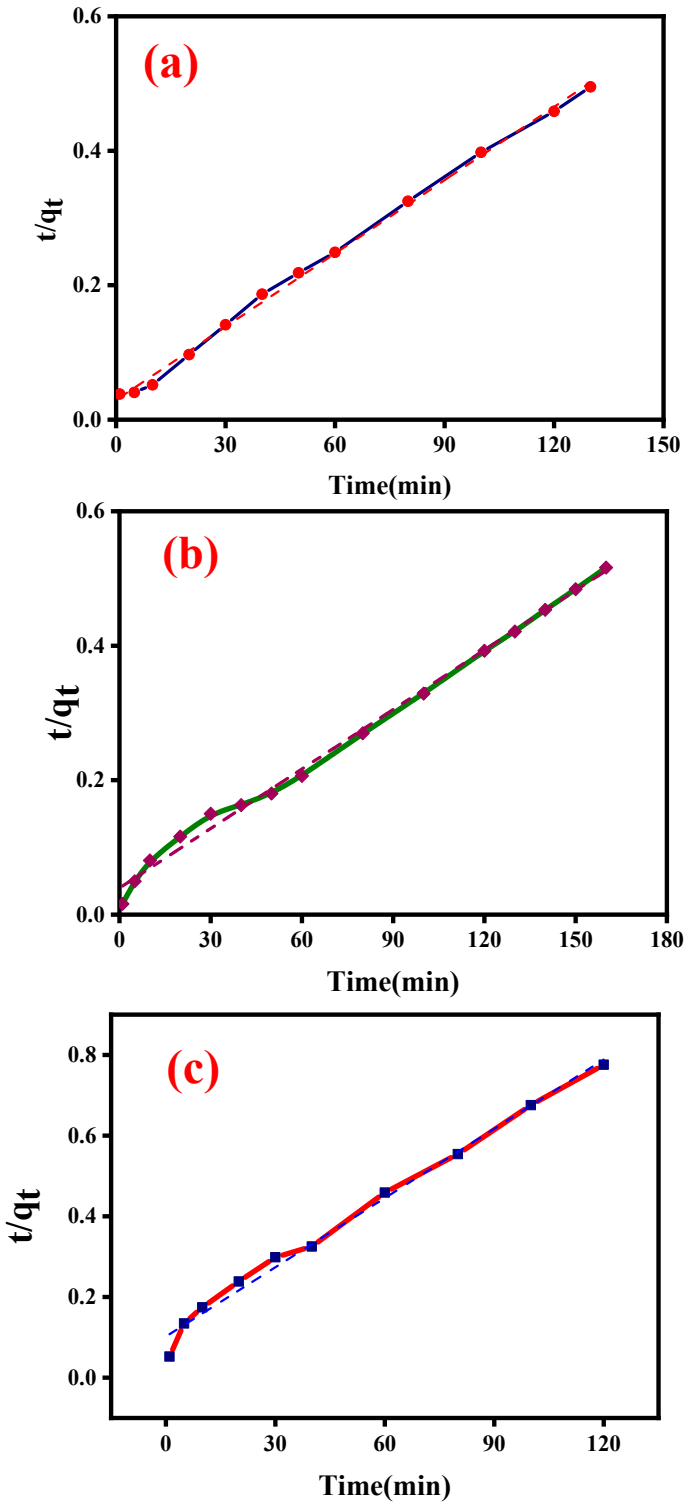


Fig. 2S. (a) Linear fitting of adsorption kinetic CIP with pseudo-second-order kinetic model fit, (b) linear fitting of adsorption kinetic MV with pseudo-second-order kinetic model fit, and (c) linear fitting of adsorption kinetic CIP+MV with pseudo-second-

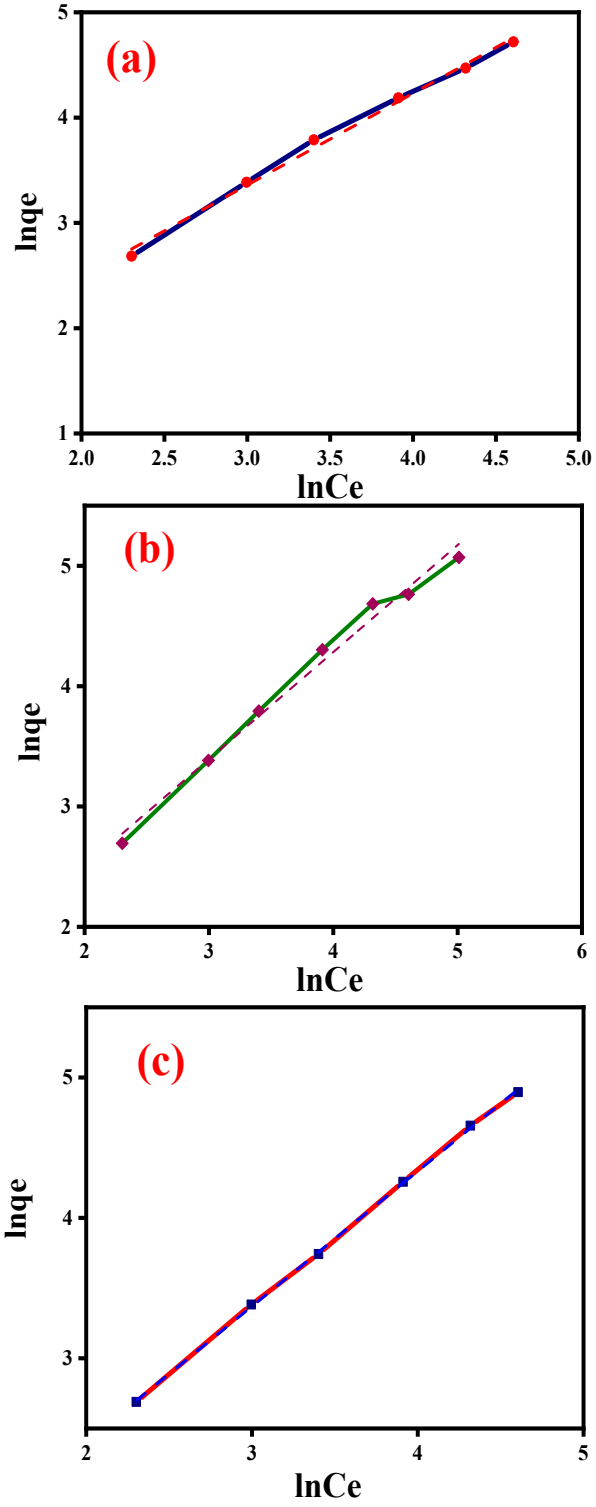


Fig. 3S.(a)Linear fitting of adsorption isotherm CIP with Freundlich isotherm model fit, (b) linear fitting of adsorption isotherm MV with Freundlich isotherm model fit and (c) linear fitting of adsorption isotherm CIP+MV with Freundlich

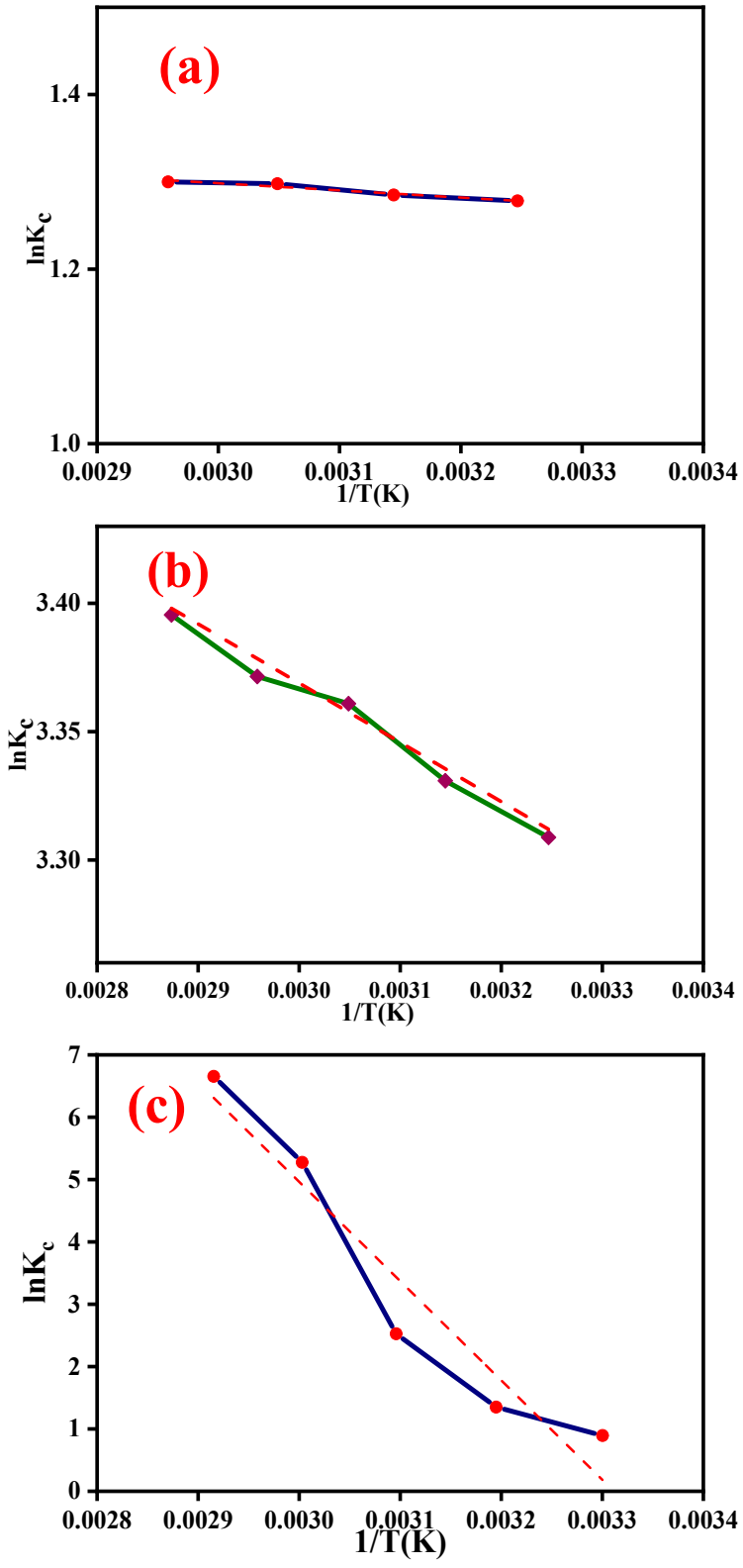


Fig. 4S. (a)-(c) linear fitting of adsorption thermodynamic CIP, CIP+MV, and MV

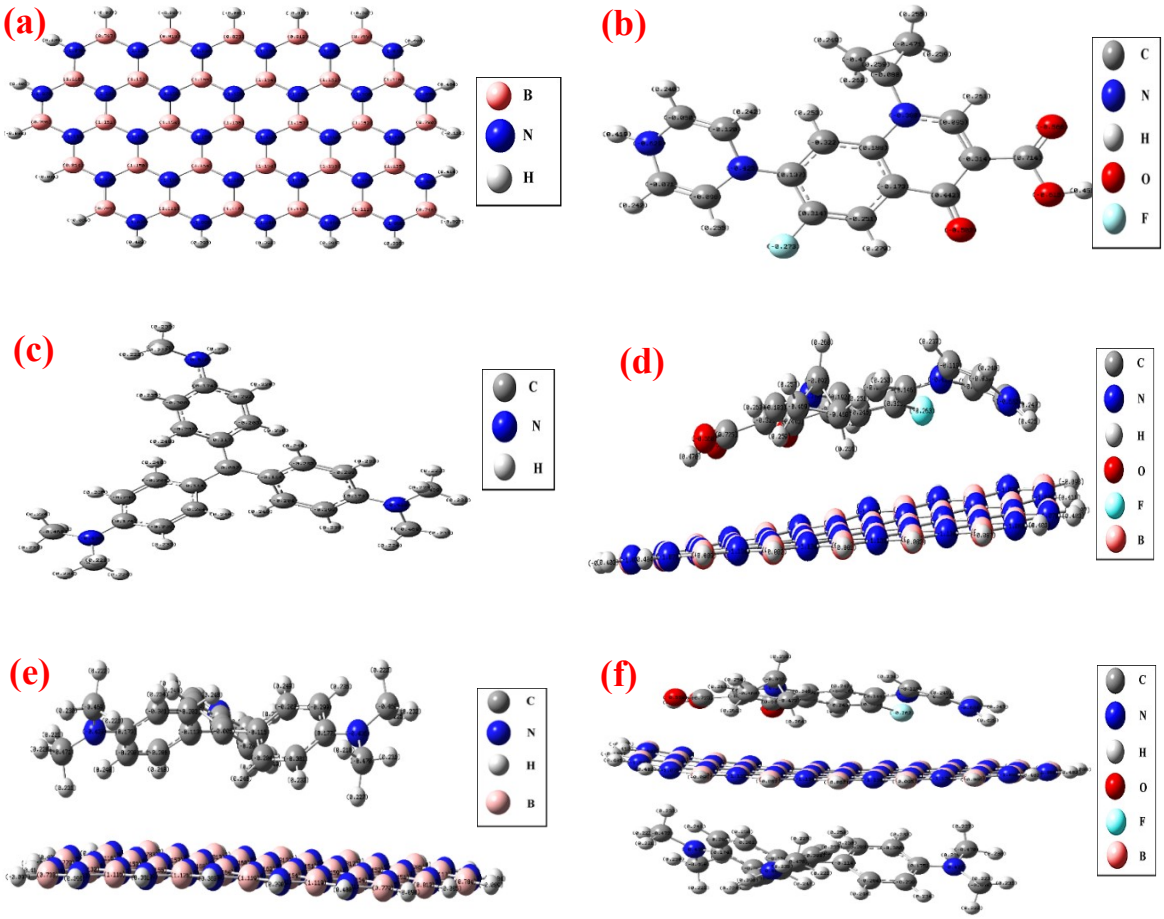


Fig. 5S. The NBO atomic charges of atoms for (a) BNNS, (b) CIP, (c) MV, (d) CIP…BN, (e) MV…BN and (f) MV…BN…CIP

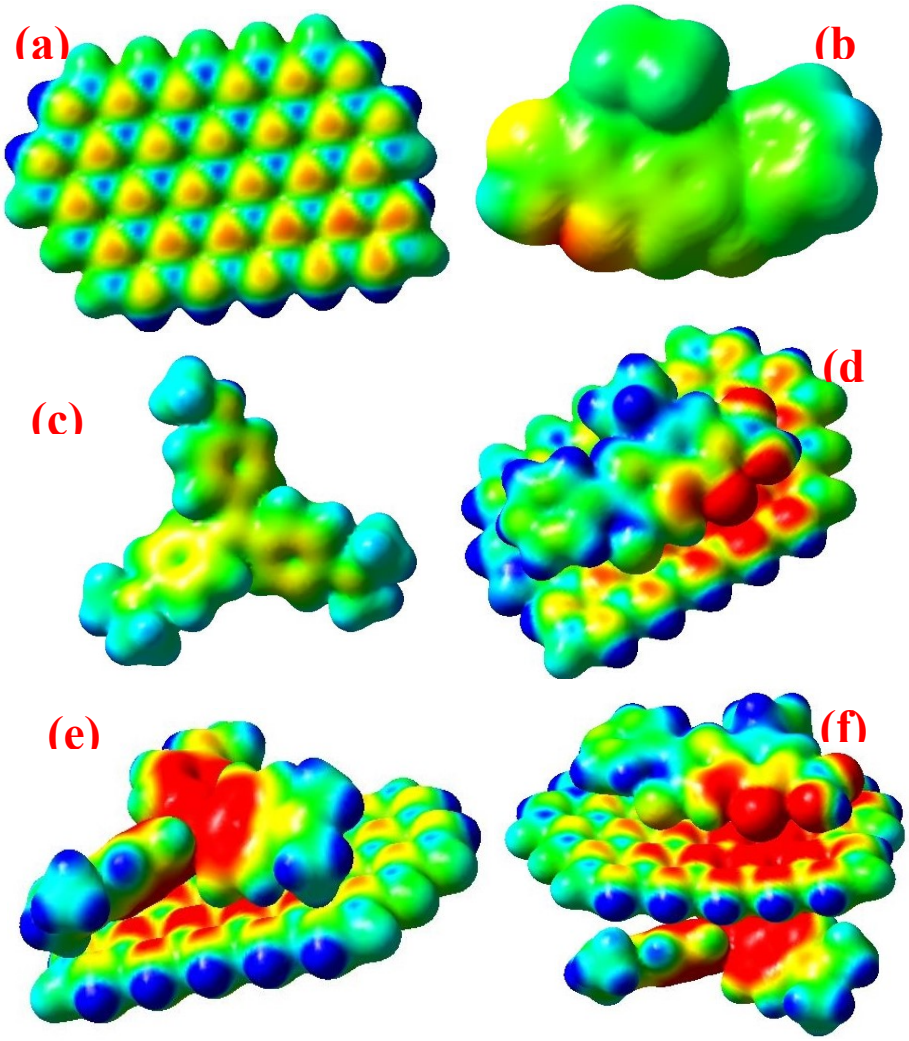
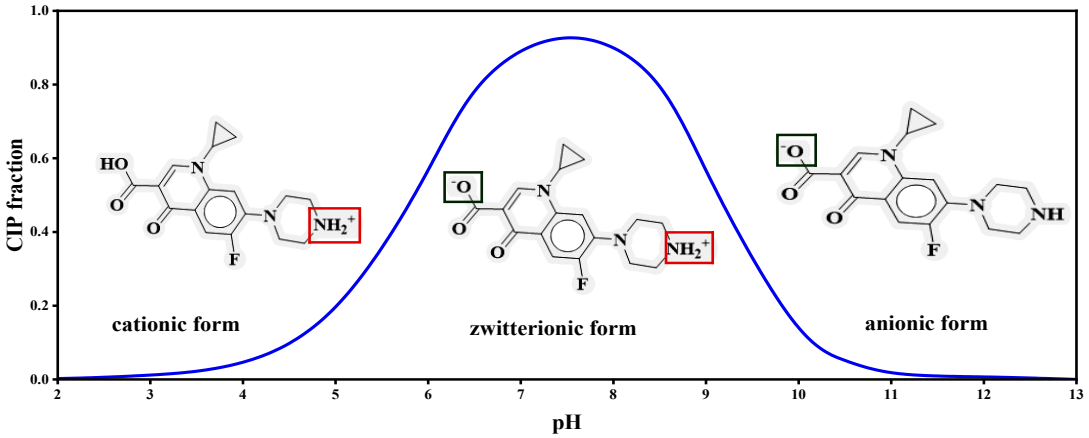


Fig.6S. The Molecular surface electrostatic potential (a) BNNS, (b) CIP, (c) MV, (d) CIP…BN, (e) MV…BN and (f) MV…BN…CIP



Molecular structure of CIP in different

Table 1S. Second order perturbation theory analysis of Fock matrix in NBO

Donor(i)	Acceptor (i)	E(2)[a](kjmol^{-1})	E(j)-E(i)[b](a.u.)	F(i,j)[c](a.u.)
CIP to BN in CIP…BN				
p F_{116}	π* B_{25}-N_{54}	5.72	0.46	0.048
p O_{111}	π* B_{28}-N_{57}	4.50	0.35	0.036
p F_{116}	π* B_{25}-N_{52}	2.62	1.12	0.052
π C_{80}- O_{91}	π* B_{27}-N_{56}	2.71	0.39	0.031
π C_{109}- O_{110}	π* B_{39}-N_{68}	1.96	0.41	0.026
π C_{85}- C_{89}	π* B_{269}-N_{55}	1.68	0.34	0.007
π C_{79}- C_{83}	π* B_{30}-N_{58}	1.53	0.33	0.020
p O_{110}	π* B_{29}-N_{70}	1.44	0.75	0.031
p O_{111}	π* B_{28}-N_{57}	1.13	0.66	0.026
p C_{81}	π* B_{31}-N_{59}	0.95	0.17	0.014
σ O_{111}- H_{112}	π* B_{28}-N_{57}	0.9	0.7	0.025
p C_{86}	π* B_{39}-N_{68}	0.75	0.17	0.012
σ H_{84}- C_{85}	π* B_{26}-N_{55}	0.65	0.58	0.019
p F_{116}	π* B_{25}-N_{53}	0.53	0.83	0.019
p F_{116}	π* B_{25}-N_{61}	0.51	0.83	0.019
BN to CIP in CIP…BN				
π B_{28}-N_{57}	σ* O_{111}- H_{112}	1.02	0.56	0.022
π B_{30}-N_{58}	π* C_{109}- O_{110}	0.98	0.24	0.014
π B_{31}-N_{59}	π* C_{80}- O_{91}	0.46	0.26	0.010
π B_{43}-N_{72}	σ* C_{92}- H_{95}	0.27	0.72	0.013
π B_{26}-N_{55}	π* C_{85}- C_{89}	0.25	0.25	0.007
π B_{40}-N_{69}	π* C_{79}- C_{83}	0.18	0.065	0.012
π B_{33}-N_{61}	π* C_{85}- C_{89}	0.10	0.27	0.005
MV to BN in MV …BN				
π C_{82}- C_{85}	π* B_{39}-N_{68}	0.57	0.32	0.016
σ C_{101}- H_{96}	π* B_{27}-N_{55}	0.49	0.59	0.007
π C_{92}- C_{95}	π* B_{27}-N_{55}	0.49	0.32	0.011
π C_{101}- C_{103}	π* B_{20}-N_{49}	0.44	0.32	0.011
π C_{92}- C_{95}	π* B_{18}-N_{47}	0.43	0.32	0.011
σ C_{101}- H_{104}	π* B_{20}-N_{49}	0.42	0.59	0.015
σ C_{82}- H_{86}	π* B_{32}-N_{60}	0.40	0.59	0.011
π C_{82}- C_{85}	π* B_{32}-N_{60}	0.439	0.32	0.010
π C_{101}- C_{103}	π* B_{21}-N_{50}	0.32	0.32	0.009
σ C_{122}- H_{123}	π* B_{17}-N_{57}	0.32	0.58	0.013
σ C_{130}- H_{131}	π* B_{43}-N_{72}	0.29	0.57	0.012
π C_{101}- C_{103}	π* B_{25}-N_{53}	0.27	0.32	0.008
σ C_{95}- H_{99}	π* B_{17}-N_{46}	0.21	0.59	0.011
BN to MV in MV …BN				
π B_{22}-N_{51}	σ* C_{114}- H_{117}	1.71	0.70	0.032
π B_{18}-N_{47}	σ* C_{122}- H_{123}	1.39	0.70	0.029
π B_{21}-N_{50}	σ* C_{103}- H_{108}	0.26	0.73	0.013
π B_{20}-N_{49}	σ* C_{101}- H_{104}	0.24	0.73	0.012
p N_{73}	σ* C_{30}- H_{131}	0.2	0.65	0.012
π B_{27}-N_{55}	π* C_{92}- C_{95}	0.14	0.26	0.005
π B_{28}-N_{56}	σ* C_{95}- H_{99}	0.14	0.71	0.010
π B_{32}-N_{60}	π* C_{82}- C_{85}	0.12	0.26	0.005
π B_{21}-N_{50}	π* C_{101}- C_{103}	0.11	0.28	0.005

BN to MV in MV…BN…CIP				
π B_{18}-N_{47}	σ* C_{122}- H_{123}	1.54	0.70	0.031
π B_{22}-N_{51}	σ* C_{114}- H_{117}	1.46	0.70	0.030
p N_{73}	σ* C_{130}- H_{131}	0.32	0.64	0.015
π B_{20}-N_{49}	σ* C_{101}- H_{104}	0.29	0.73	0.014
π B_{21}-N_{50}	σ* C_{103}- H_{108}	0.26	0.73	0.013
π B_{28}-N_{56}	σ* C_{95}- H_{99}	0.22	0.70	0.012
π B_{27}-N_{55}	π* C_{92}- C_{95}	0.20	0.26	0.006
π B_{32}-N_{60}	π* C_{82}- C_{85}	0.17	0.26	0.006
MV to BN in MV…BN…CIP				
σ C_{92}- H_{96}	π* B_{27}-N_{55}	0.66	0.06	0.019
π C_{92}- C_{95}	π* B_{27}-N_{55}	0.54	0.33	0.012
π C_{101}- C_{103}	π* B_{20}-N_{49}	0.50	0.32	0.011
π C_{82}- C_{85}	π* B_{39}-N_{68}	0.49	0.32	0.010
π C_{92}- C_{95}	π* B_{18}-N_{47}	0.44	0.33	0.011
σ C_{101}- H_{104}	π* B_{20}-N_{49}	0.45	0.59	0.016
σ C_{82}- H_{86}	π* B_{39}-N_{68}	0.41	0.59	0.008
π C_{82}- C_{85}	π* B_{32}-N_{60}	0.40	0.32	0.010
σ C_{82}- H_{86}	σ* B_{25}	0.31	0.27	0.009
π C_{101}- C_{103}	π* B_{21}-N_{50}	0.30	0.31	0.009
σ C_{95}- H_{99}	π* B_{18}-N_{47}	0.25	0.60	0.007
BN to CIP in MV…BN…CIP				
π B_{19}-N_{48}	π* C_{164}- O_{165}	0.69	0.25	0.0012
π B_{18}-N_{47}	σ* O_{166}- H_{167}	0.59	0.57	0.017
π B_{27}-N_{55}	π* C_{135}- O_{146}	0.21	0.26	0.007
π B_{37}-N_{66}	π* C_{156}- C_{159}	0.18	0.27	0.006
π B_{38}-N_{67}	π* C_{140}- C_{144}	0.17	0.28	0.006
π B_{31}-N_{61}	π* C_{140}- C_{144}	0.15	0.26	0.006
CIP to BN in MV…BN…CIP				
p F_{171}	π* B_{39}-N_{68}	6.09	0.45	0.049
p O_{166}	π* B_{18}-N_{47}	4.85	0.35	0.038
π C_{135}- C_{146}	π* B_{27}-N_{55}	3.49	0.38	0.035
p F_{171}	π* B_{39}-N_{68}	2.54	1.11	0.051
p O_{146}	π* B_{27}-N_{55}	1.79	0.74	0.035
π C_{140}- C_{144}	π* B_{31}-N_{59}	1.29	0.33	0.019
p O_{166}	π* B_{18}-N_{47}	1.14	0.66	0.026
p C_{136}	π* B_{26}-N_{54}	1.05	0.16	0.014
σ O_{166}- H_{167}	π* B_{18}-N_{47}	0.93	0.77	0.026
π C_{134}- C_{138}	π* B_{19}-N_{48}	0.92	0.33	0.016
π C_{143}- N_{169}	π* B_{38}-N_{67}	0.79	0.37	0.016
p F_{171}	π* B_{39}-N_{73}	0.78	0.81	0.023
σ C_{156}- H_{160}	π* B_{33}-N_{61}	0.69	0.59	0.019
σ H_{139}- C_{140}	π* B_{33}-N_{61}	0.67	0.57	0.019
π C_{156}- C_{159}	π* B_{37}-N_{66}	0.65	0.33	0.014
p O_{146}	π* B_{30}-N_{57}	0.62	0.73	0.020
p F_{171}	π* B_{39}-N_{73}	0.52	1.48	0.025
π C_{144}- F_{171}	π* B_{39}-N_{68}	0.50	1.01	0.022
π C_{140}- C_{144}	π* B_{32}-N_{60}	0.50	0.32	0.011
π C_{135}- O_{146}	π* B_{27}-N_{59}	0.48	0.76	0.017

[a] *E* (2): Energy of hyperconjugative interaction (stabilization energy).
[b] Energy difference between donor and acceptor I and j NBO orbitals.
[c] *F* (*i*,*j*): The fork matrix element between I and j NBO orbitals.