Supporting Information

Carbon and boron nitride quantum dots as optical sensor probes for selective detection of toxic metals in drinking water: A quantum chemical prediction through structural and morphological dependent electronic and optical properties

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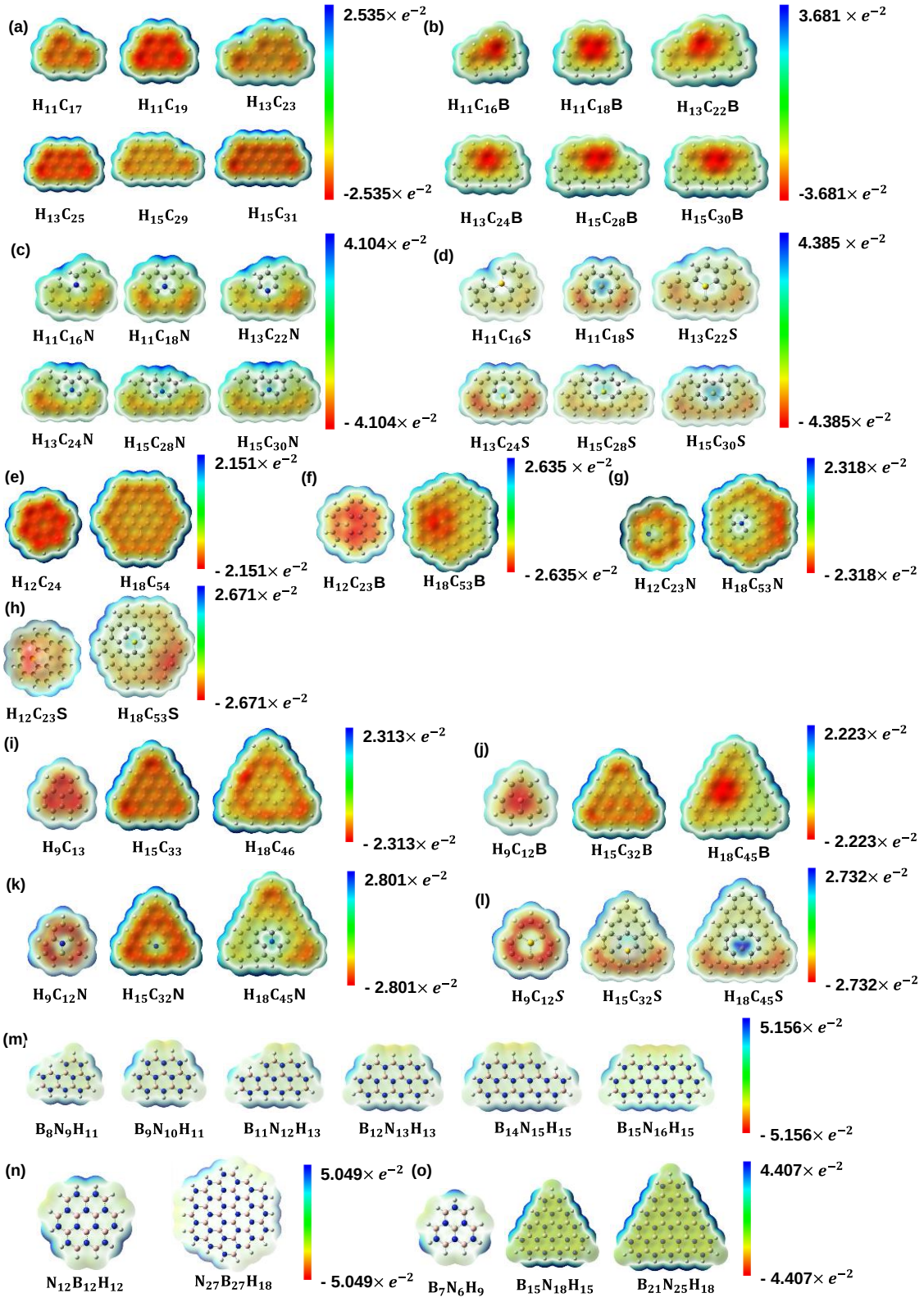

Figure S1. ESP plot of rectangular (a) CQDs, (b) boron-doped CQDs, (c) nitrogen-doped CQDs, (d) sulphur-doped CQDs; Circular (e) CQDs, (f) boron-doped CQDs, (g) nitrogen-doped CQDs, (h) sulphur-doped CQDs; Triangular (i) CQDs, (j) boron-doped CQDs, (k) nitrogen-doped CQDs, (l) sulphur doped CQDs; (m) rectangular BNQD, (n) circular BNQD, (o) triangular BNQD.

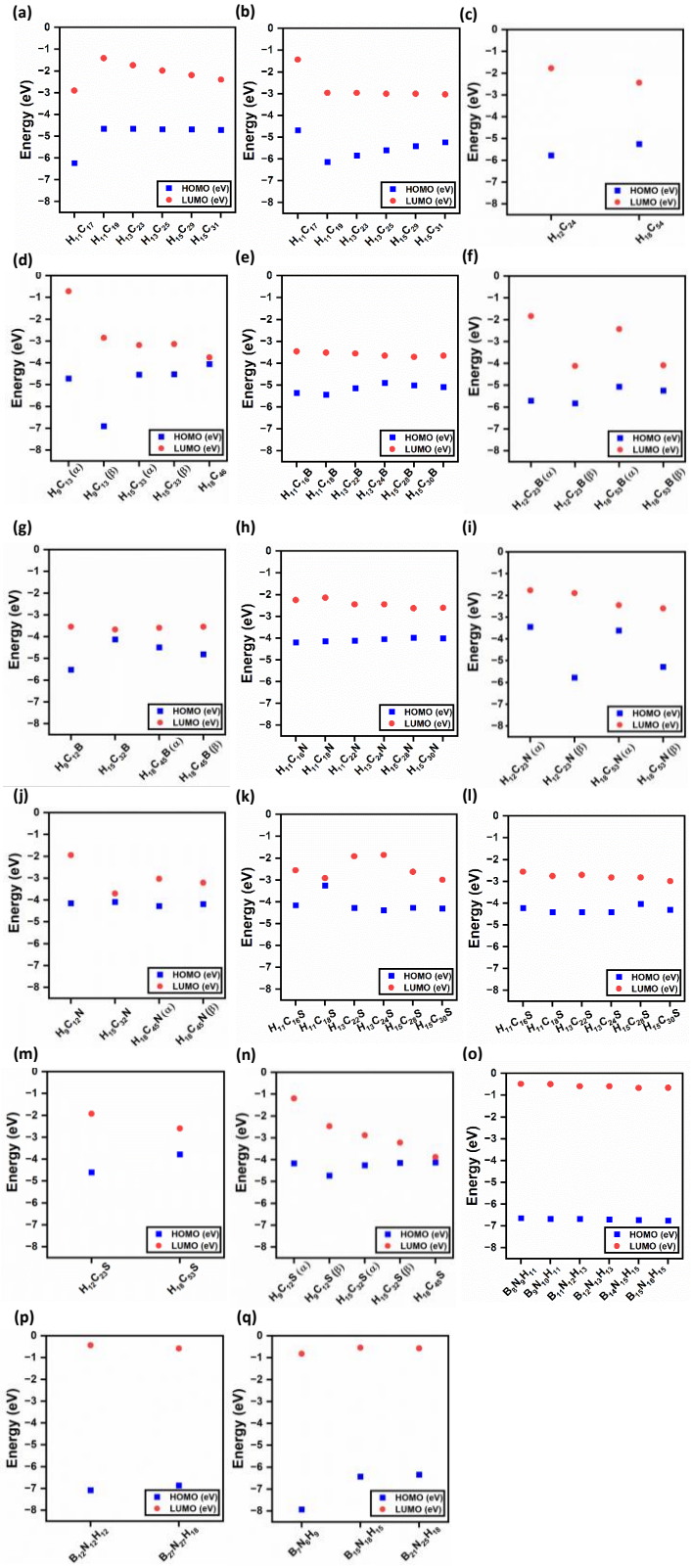

Figure S2. HOMO-LUMO plot of rectangular (a) alpha molecular orbitals of CQDs, (b) beta molecular orbitals of CQDs; (c) circular CQDs; (d) triangular CQDs; (e) rectangular B-doped CQDs; (f) circular B-doped CQDs; (g) triangular B-doped CQDs; (h) rectangular N-doped CQDs; (i) circular N-doped CQDs; (j) triangular N-doped CQDs; (k) alpha molecular orbitals of sulphur doped CQDs, (l) beta molecular orbitals of sulphur doped CQDs; (m) circular S-doped CQDs; (n) triangular S-doped CQDs; (o) rectangular BNQDs; (p) circular BNQDs; (q) triangular BNQDs.

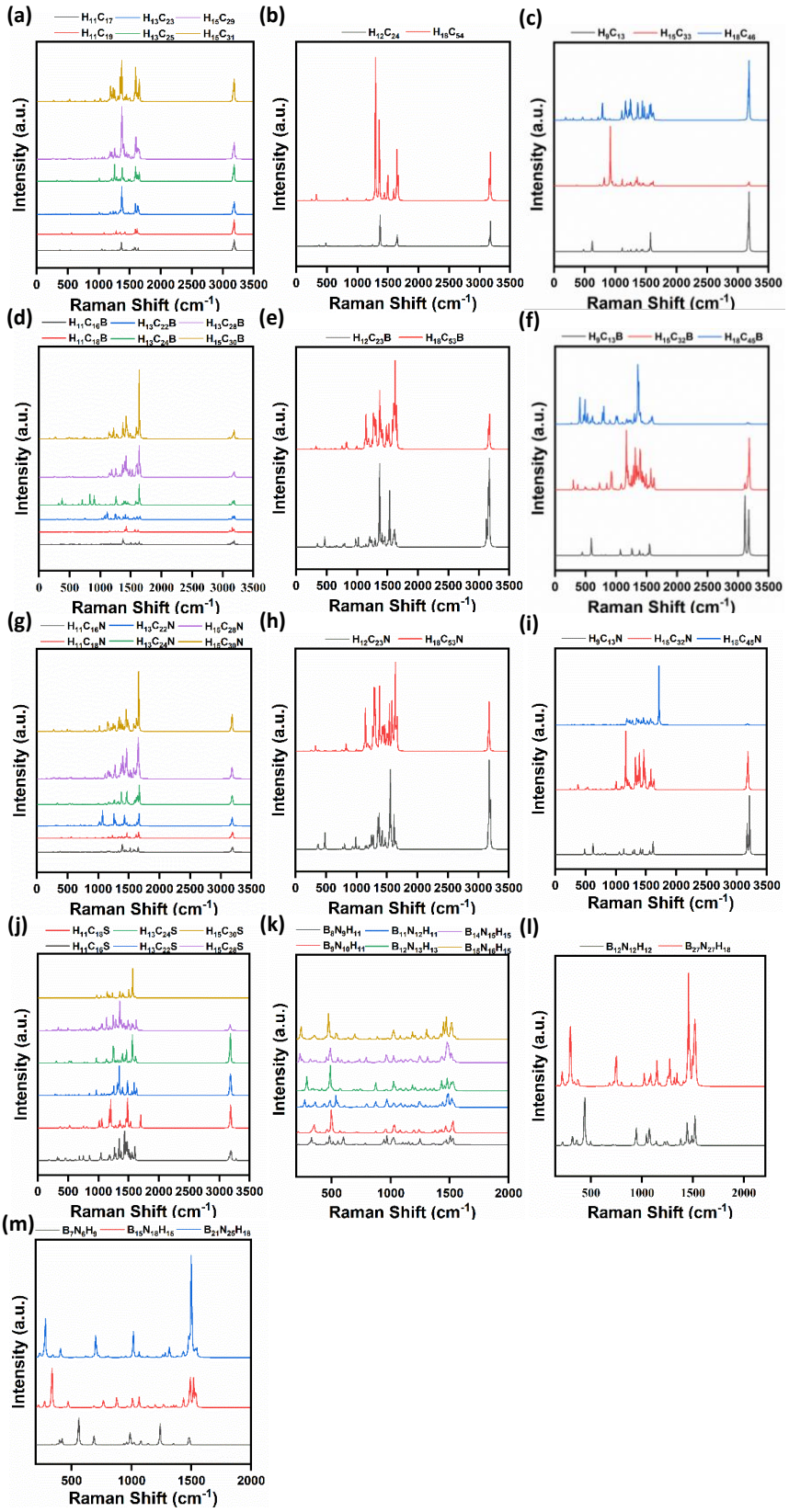

Figure S3. Raman Spectra plots of (a) rectangular CQDs, (b) circular CQDs, (c) triangular CQDs; Boron doped (d) rectangular CQDs, (e) circular CQDs, (f) triangular CQDs; Nitrogen doped (g) rectangular CQDs, (h) circular CQDs, (i) triangular CQDs; Sulphur doped (j) rectangular CQDs, (k) rectangular BNQDs, (l) circular BNQDs, (m) triangular BNQDs.

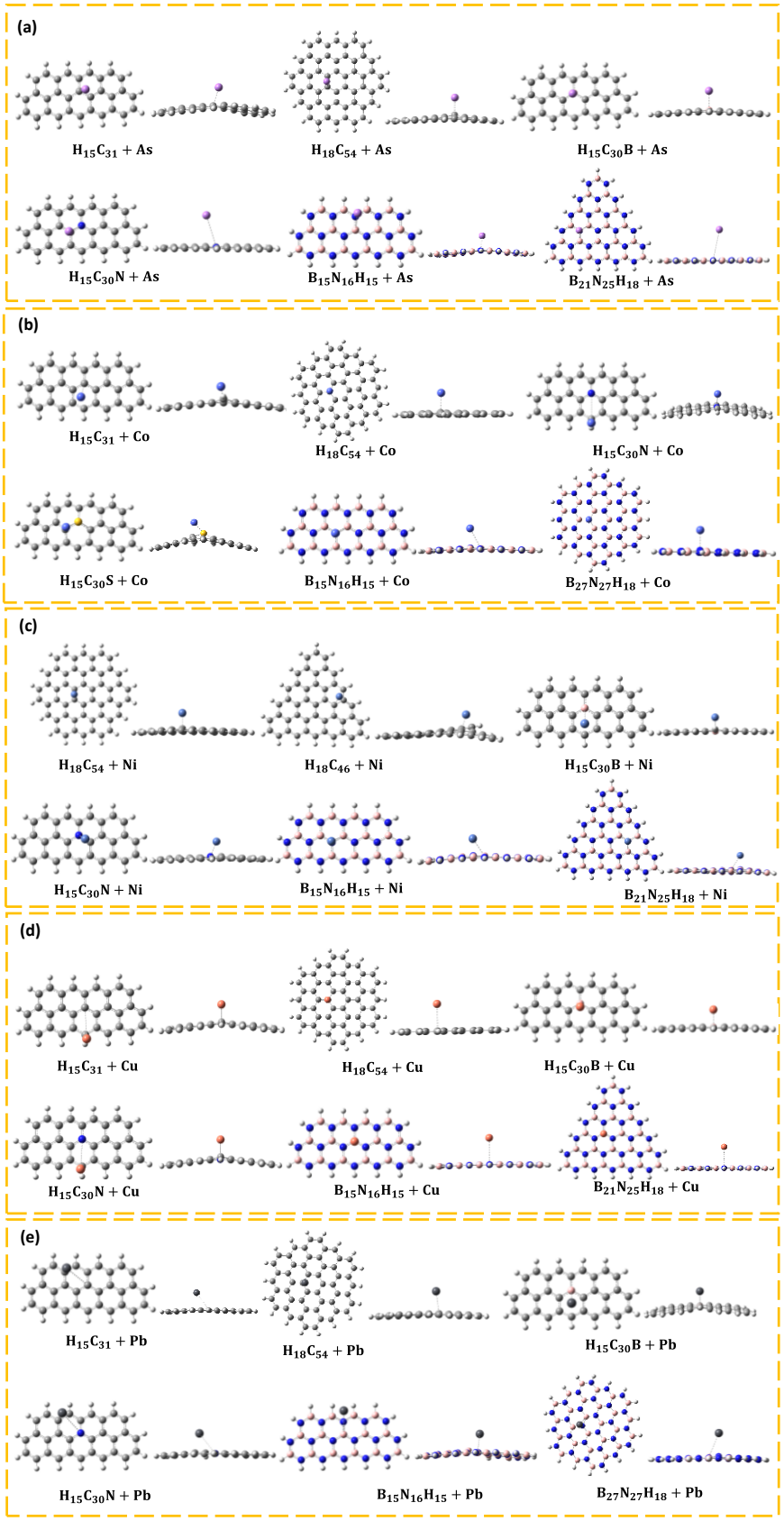

Figure S4. Optimized structures of QDs with metals (a) As, (b) Co, (c) Ni, (d) Cu, and (e) Pb.

Table S1. Formation energies of QDs with toxic metals in gas and water phases.

Morphology/QD	Formation energy (eV)									
	Gas phase					Water Phase				
	As	Co	Ni	Cu	Pb	As	Co	Ni	Cu	Pb
Rectangular $H_{15}C_{31}$	-5.97	-5.96	-6.02	-5.99	-5.99	-6.65	-6.65	-6.72	-6.68	-6.67
Circular $H_{18}C_{54}$	-7.30	-7.29	-7.31	-7.29	-7.29	-7.21	-7.22	-7.23	-7.21	-7.21
Triangular $H_{18}C_{46}$	-7.07	-7.04	-7.06	-7.04	-7.04	-6.98	-6.97	-6.99	-6.96	-6.97
Rectangular $H_{15}C_{30}B$	-5.92	-5.92	-5.93	-5.91	-5.94	-6.60	-6.62	-6.63	-6.60	-6.62
Rectangular $H_{15}C_{30}N$	-5.94	-5.93	-5.94	-5.93	-5.93	-6.62	-6.63	-6.64	-6.62	-6.62
Rectangular $H_{15}C_{30}S$	-5.79	-5.80	-5.82	-5.81	-5.80	-6.48	-6.46	-6.52	-6.50	-6.48
Rectangular $B_{15}N_{16}H_{15}$	-6.03	-6.01	-6.04	-6.01	-6.02	-6.00	-5.98	-6.01	-5.98	-5.98
Circular $B_{27}N_{27}H_{18}$	-6.47	-6.46	-6.48	-6.46	-6.46	-6.43	-6.42	-6.45	-6.43	-6.43
Triangular $B_{21}N_{25}H_{18}$	-6.38	-6.37	-6.38	-6.37	-6.37	-6.35	-6.34	-6.36	-6.34	-6.34

Table S2. Details on dipole moment of QD before and after metals adsorption.

QD	Dipole moment (Debye)	Complex	Dipole moment (Debye)
Rectangular $H_{15}C_{31}$	0.004	$H_{15}C_{31}$+As	1.57
		$H_{15}C_{31}$+Co	2.21
		$H_{15}C_{31}$+Ni	2.55
		$H_{15}C_{31}$+Cu	2.07
		$H_{15}C_{31}$+Pb	0.74
Circular $H_{18}C_{54}$	0.000052	$H_{18}C_{54}$+As	1.01
		$H_{18}C_{54}$+Co	1.84
		$H_{18}C_{54}$+Ni	1.56
		$H_{18}C_{54}$+Cu	0.77
		$H_{18}C_{54}$+Pb	0.72
Triangular $H_{18}C_{46}$	0.000111	$H_{18}C_{46}$+As	0.04
		$H_{18}C_{46}$+Co	0.67
		$H_{18}C_{46}$+Ni	2.94
		$H_{18}C_{46}$+Cu	1.12
		$H_{18}C_{46}$+Pb	4.07
Rectangular $H_{15}C_{30}B$	3.13	$H_{15}C_{30}B$+As	0.22
		$H_{15}C_{30}B$+Co	3.53
		$H_{15}C_{30}B$+Ni	3.68
		$H_{15}C_{30}B$+Cu	3.26
		$H_{15}C_{30}B$+Pb	4.04
Rectangular $H_{15}C_{30}N$	3.35	$H_{15}C_{30}N$+As	2.47
		$H_{15}C_{30}N$+Co	1.13
		$H_{15}C_{30}N$+Ni	3.78
		$H_{15}C_{30}N$+Cu	1.43
		$H_{15}C_{30}N$+Pb	4.98
Rectangular $H_{15}C_{30}S$	2.47	$H_{15}C_{30}S$+As	4.50
		$H_{15}C_{30}S$+Co	3.55
		$H_{15}C_{30}S$+Ni	0.91

		$H_{15}C_{30}S$+Cu	2.89
		$H_{15}C_{30}S$+Pb	0.80
Rectangular $B_{15}N_{16}H_{15}$	4.31	$B_{15}N_{16}H_{15}$+As	5.17
		$B_{15}N_{16}H_{15}$+Co	4.81
		$B_{15}N_{16}H_{15}$+Ni	4.41
		$B_{15}N_{16}H_{15}$+Cu	4.31
		$B_{15}N_{16}H_{15}$+Pb	3.91
Circular $B_{27}N_{27}H_{18}$	0.002976	$B_{27}N_{27}H_{18}$+As	0.11
		$B_{27}N_{27}H_{18}$+Co	2.11
		$B_{27}N_{27}H_{18}$+Ni	0.33
		$B_{27}N_{27}H_{18}$+Cu	0.39
		$B_{27}N_{27}H_{18}$+Pb	0.81
Triangular $B_{21}N_{25}H_{18}$	0.002776	$B_{21}N_{25}H_{18}$+As	0.03
		$B_{21}N_{25}H_{18}$+Co	2.58
		$B_{21}N_{25}H_{18}$+Ni	0.22
		$B_{21}N_{25}H_{18}$+Cu	0.72
		$B_{21}N_{25}H_{18}$+Pb	3.19