Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A quasi-plane IrB_{18}^- cluster with high stability

Donghe Wei,[a] Mengxue Ren,[a] Cheng Lu,[*a,b] Jie Bi,[*b] and George Maroulis[*c]

[a]*Department of Physics and Optoelectronic Engineering, Yangtze University, Jingzhou 434023, China*

[b]*School of Mathematics and Physics, China University of Geosciences (Wuhan), Wuhan 430074, China*

[c]*Department of Chemistry, University of Patras, GR-26500 Patras, Greece*

Cheng Lu

*E-mail: lucheng@calypso.cn

Jie Bi

*E-mail: bijiecug@163.com

George Maroulis

*E-mail: maroulis@upatras.gr

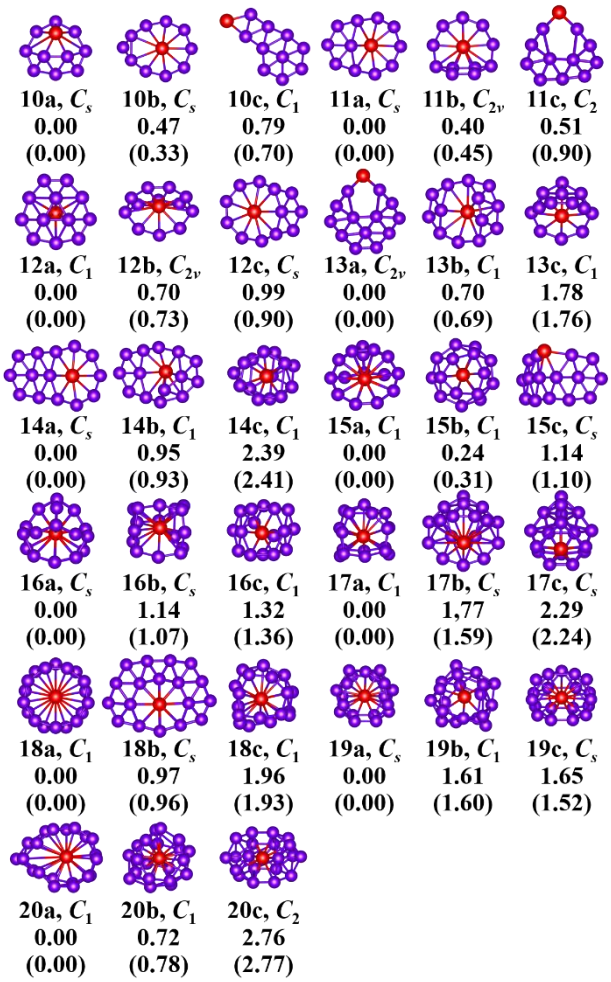

Figure S1. The lowest energy and metastable isomers of neutral IrB_n (n=10−20) at PBE0/Ir/LANL2DZ/B/6-311+G(d) and PBE0/Ir/LANL2DZ/B/6-311+G(d) with correction for Gibbs free energy, which is shown in the parenthesis.

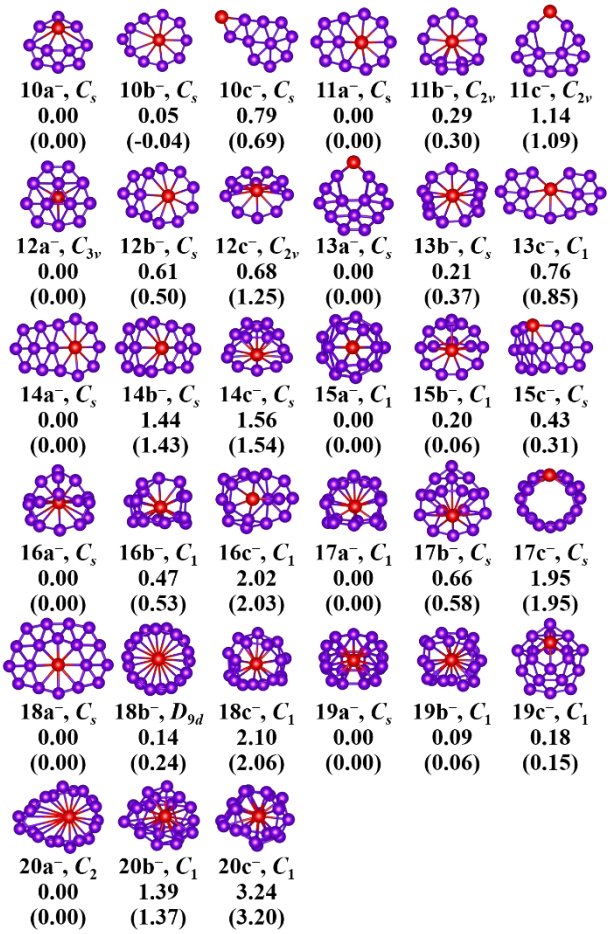

Figure S2. The lowest energy and metastable isomers of anionic IrB_n^- (n=10−20) at PBE0/Ir/LANL2DZ/B/6-311+G(d) and PBE0/Ir/LANL2DZ/B/6-311+G(d) with correction for Gibbs free energy, which is shown in the parenthesis.

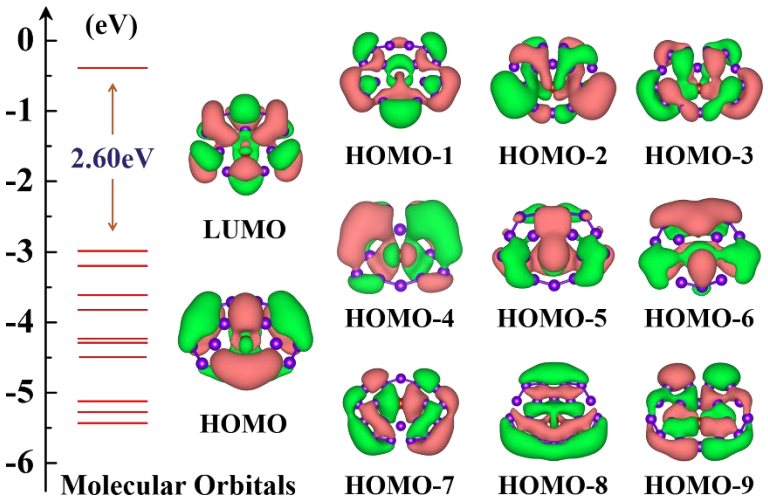

Figure S3. MOs of the IrB_{18}^- cluster.

Table S1. The energy of IrB_{18}^- calculated at different calculation levels.

Isomers	E (a. u.)	
	PBE0/Ir/LANL2DZ/B/6-311+G(d)	CCSD(T)/Ir/Stuttgart/B/6-311+G(d)
$18a^-$	-551.4367484	-549.4522894
$18b^-$	-551.4316093	-549.4446119
$18c^-$	-551.359686	-549.39499727

Table S2. The calculated electronic states, NPA charges, E_b, E_{gap} and VDE of the lowest energy structures of the $IrB_n^{0/-}$ (n = 10−20) clusters.

	IrB_n				IrB_n^-				
n	State	Q(Ir)	E_b	E_{gap}	State	Q(Ir)	E_b	E_{gap}	VDE
10	^{2}A'	0.06	4.92	2.27	^{1}A'	−0.18	5.18	2.72	3.35
11	^{1}A'	−0.21	5.02	2.60	^{2}A'	−0.32	5.28	1.91	3.61
12	^{2}A	0.10	5.10	1.90	^{1}A$_1$	−0.11	5.34	3.30	3.41
13	^{1}A$_1$	−0.23	5.10	3.07	^{2}A"	−0.40	5.24	1.45	2.58
14	^{2}A"	−0.42	5.14	1.94	^{1}A$_1$	−0.44	5.38	2.28	3.92
15	^{1}A	−0.97	5.15	3.60	^{2}A	−0.67	5.31	1.98	3.46
16	^{2}A'	−0.94	5.17	2.00	^{1}A'	−1.04	5.35	3.35	3.53
17	^{1}A	−1.33	5.25	3.63	^{2}A	−1.06	5.36	1.81	2.89
18	^{2}A	−0.53	5.30	1.54	^{1}A'	−0.32	5.46	2.60	4.25
19	^{1}A'	−1.42	5.24	3.95	^{2}A'	−0.70	5.32	1.77	4.31
20	^{2}A	−0.51	5.24	1.62	^{1}A	−0.50	5.45	1.95	3.34