

Supporting Information

Structure and Bonding of IrB₁₂⁻: Converting a Rigid Boron B₁₂ Platelet to a Wankel Motor

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Cartesian coordinates

$\text{B}_{12} \text{ (GM, } C_{3v})$

0 1

B	0.485840	0.841500	0.390993
B	0.485840	-0.841500	0.390993
B	-1.007898	-1.745731	-0.039718
B	-2.295639	-0.776110	-0.175638
B	-0.971681	0.000000	0.390993
B	-1.007898	1.745731	-0.039718
B	-2.295639	0.776110	-0.175638
B	0.475689	-2.376137	-0.175638
B	2.015796	0.000000	-0.039718
B	1.819951	1.600027	-0.175638
B	0.475689	2.376137	-0.175638
B	1.819951	-1.600027	-0.175638

$\text{CoB}_{12}^- \text{ (GM, } C_{3v})$

-1 1

Co	0.000000	0.000000	0.729114
B	-1.760827	1.016614	-0.241077
B	-0.764073	2.207359	-0.038899
B	-2.293665	-0.441973	-0.038899
B	1.760827	1.016614	-0.241077
B	0.000000	-2.033228	-0.241077
B	1.529592	-1.765386	-0.038899
B	-1.529592	-1.765386	-0.038899
B	2.293665	-0.441973	-0.038899
B	0.764073	2.207359	-0.038899
B	0.850665	-0.491131	-0.987427
B	0.000000	0.982263	-0.987427
B	-0.850665	-0.491131	-0.987427

$\text{RhB}_{12}^- \text{ (GM, } C_{3v})$

-1 1

Rh	0.000000	0.000000	0.877788
B	-1.782770	1.029283	-0.252116
B	-0.771386	2.237896	-0.073200
B	-2.323768	-0.450908	-0.073200
B	1.782770	1.029283	-0.252116
B	0.000000	-2.058566	-0.252116
B	1.552382	-1.786988	-0.073200
B	-1.552382	-1.786988	-0.073200
B	2.323768	-0.450908	-0.073200
B	0.771386	2.237896	-0.073200
B	0.854456	-0.493320	-0.957617
B	0.000000	0.986641	-0.957617
B	-0.854456	-0.493320	-0.957617

IrB₁₂⁻ (GM, C_{3v})

-1 1

Ir	0.000000	0.000000	0.834517
B	-1.803319	1.041147	-0.238175
B	-0.771906	2.227873	-0.052332
B	-2.315347	-0.445447	-0.052332
B	1.803319	1.041147	-0.238175
B	0.000000	-2.082294	-0.238175
B	1.543442	-1.782426	-0.052332
B	-1.543442	-1.782426	-0.052332
B	2.315347	-0.445447	-0.052332
B	0.771906	2.227873	-0.052332
B	0.859656	-0.496323	-0.998859
B	0.000000	0.992645	-0.998859
B	-0.859656	-0.496323	-0.998859

B₁₂ (TS, C_{3v})

0 1

B	-0.484070	-0.838440	0.464163
B	-0.484070	0.838440	0.464163

B	-2.085810	0.807630	-0.139978
B	-1.222550	2.117510	-0.184208
B	0.968150	0.000000	0.464163
B	1.742330	1.402550	-0.139978
B	0.343480	2.210180	-0.139978
B	-2.085810	-0.807630	-0.139978
B	0.343480	-2.210180	-0.139978
B	1.742330	-1.402550	-0.139978
B	2.445090	0.000000	-0.184208
B	-1.222550	-2.117510	-0.184208

CoB₁₂⁻ (TS, C_{3v})

-1 1

B	-0.490182	-0.849018	0.782591
B	-0.490179	0.849020	0.782591
B	-2.055928	0.780350	-0.128519
B	-1.180574	2.044823	-0.213999
B	0.980363	-0.000002	0.782591
B	1.703768	1.390312	-0.128519
B	0.352170	2.170660	-0.128519
B	-2.055931	-0.780343	-0.128519
B	0.352162	-2.170662	-0.128519
B	1.703763	-1.390318	-0.128519
B	2.361156	-0.000004	-0.213999
B	-1.180581	-2.044819	-0.213999
Co	0.000000	0.000000	-0.934659

RhB₁₂⁻ (TS, C_{3v})

-1 1

B	-0.493009	-0.853910	0.760968
B	-0.493003	0.853914	0.760968
B	-2.078920	0.790420	-0.108412
B	-1.195373	2.070464	-0.187092
B	0.986013	-0.000003	0.760968

B	1.723984	1.405188	-0.108412
B	0.354951	2.195605	-0.108412
B	-2.078925	-0.790406	-0.108412
B	0.354936	-2.195608	-0.108412
B	1.723974	-1.405199	-0.108412
B	2.390761	-0.000008	-0.187092
B	-1.195387	-2.070456	-0.187092
Rh	0.000000	0.000000	-1.071162

IrB₁₂⁻ (TS, C_{3v})

-1 1

B	-0.496637	-0.860207	0.798692
B	-0.496641	0.860205	0.798692
B	-2.084179	0.789913	-0.122809
B	-1.191022	2.062903	-0.208254
B	0.993282	0.000002	0.798692
B	1.726176	1.409996	-0.122809
B	0.357997	2.199911	-0.122809
B	-2.084175	-0.789922	-0.122809
B	0.358007	-2.199909	-0.122809
B	1.726182	-1.409989	-0.122809
B	2.382039	0.000005	-0.208254
B	-1.191013	-2.062908	-0.208254
Ir	0.000001	0.000000	-1.034521

IrB₁₂⁻ (2, C_s)

-1 1

Ir	-0.350626	0.045064	0.128847
B	-0.398040	2.052829	-1.205764
B	0.739304	-1.434693	1.418114
B	1.150286	-1.428113	-0.476491
B	1.105545	1.529999	-0.551658
B	0.873423	0.106946	1.847437
B	0.231268	-0.818884	-1.934565

B	-0.085346	2.461152	0.284048
B	-0.336030	-2.028656	-1.101454
B	1.563563	0.046357	-0.948828
B	0.693102	1.619915	1.339836
B	-0.012074	-2.351624	0.406674
B	0.206837	0.819533	-1.975585

IrB₁₂⁻ (3, C₂)

-1 1

Ir	0.000000	0.000000	0.502622
B	0.100780	2.290570	-0.056468
B	-0.667560	-1.158060	-1.273398
B	-0.100780	-2.290570	-0.056468
B	0.218770	0.747440	2.502872
B	0.667560	1.158060	-1.273398
B	-0.439210	-1.886300	1.445302
B	-0.872830	0.342810	-1.712928
B	0.872830	-0.342810	-1.712928
B	0.439210	1.886300	1.445302
B	-0.218770	-0.747440	2.502872
B	0.918200	-1.847860	-1.156688
B	-0.918200	1.847860	-1.156688

IrB₁₂⁻ (4, C_s)

-1 1

Ir	-0.000071	-0.372258	0.001547
B	-1.632974	1.419768	-0.105420
B	0.000608	3.682971	0.099017
B	-2.088993	-0.002740	-0.542607
B	-1.887658	-1.495311	-0.240170
B	0.766931	-2.416429	0.277946
B	1.887122	-1.495979	-0.240183
B	2.088967	-0.003480	-0.542643
B	0.000294	1.990426	-0.205395

B	-1.342737	2.937549	0.218444
B	1.633364	1.419199	-0.105570
B	1.343695	2.937075	0.218376
B	-0.767767	-2.416196	0.277848

IrB₁₂⁻ (5, C_s)

-1 1

Ir	-0.028943	-0.195975	-0.077018
B	-2.192338	-0.347472	0.437680
B	2.052201	-0.834892	0.403960
B	-1.315417	1.993133	-0.658785
B	-0.288674	-2.454046	-0.148212
B	0.963083	1.583657	0.973394
B	2.294227	0.719844	0.424382
B	1.172367	-2.059646	0.041988
B	1.710911	1.644004	-0.680519
B	-1.619096	-1.739617	0.066218
B	-0.576663	1.762878	0.983682
B	-2.075838	1.221667	0.455555
B	0.235221	2.146856	-0.730725

IrB₁₂⁻ (6, C_{2v})

-1 1

Ir	0.000000	0.000000	0.111800
B	0.000000	2.375841	-0.438195
B	1.259278	1.473129	-0.929205
B	-1.259278	1.473129	-0.929205
B	0.000000	1.957170	1.109378
B	0.000000	-0.765650	2.163250
B	0.000000	-1.957170	1.109378
B	0.000000	-2.375841	-0.438195
B	1.259278	-1.473129	-0.929205
B	-1.259278	-1.473129	-0.929205
B	1.795649	0.000000	-1.031988

B	-1.795649	0.000000	-1.031988
B	0.000000	0.765650	2.163250

IrB₁₂⁻ (7, C_s)

-1 1

Ir	0.000000	0.000000	1.592800
B	0.000000	-2.010860	1.894040
B	0.000000	-2.865790	-0.785470
B	0.000000	1.574840	0.220880
B	0.000000	2.010860	1.894040
B	0.000000	0.000000	-0.443750
B	0.000000	2.865790	-0.785470
B	0.000000	3.142240	0.733000
B	0.000000	-1.574840	0.220880
B	0.000000	-3.142240	0.733000
B	0.000000	0.000000	-2.143870
B	0.000000	-1.449720	-1.565040
B	0.000000	1.449720	-1.565040

IrB₁₂⁻ (8, C_s)

-1 1

Ir	-0.515241	0.236437	-0.055639
B	-1.230298	-1.006100	-1.579907
B	-1.447469	-1.010991	1.338804
B	2.649931	-0.229490	1.817317
B	2.865160	-0.220021	0.202124
B	0.112444	-0.337812	-2.127265
B	2.894913	-0.214082	-1.429453
B	1.275969	-0.084590	0.953091
B	1.405832	-0.085260	-0.781272
B	-1.894073	-1.290310	-0.162617
B	1.700661	-0.156795	-2.405345
B	1.322522	-0.169511	2.603404
B	-0.205342	-0.339148	2.085186

IrB₁₂⁻ (9, C_{2v})**-1 1**

Ir	-0.066784	-0.439644	-0.000188
B	0.053017	-1.970635	1.467236
B	0.052905	-1.969942	-1.468379
B	-0.332730	2.465187	-1.141544
B	-0.178418	0.977384	-1.697690
B	-0.178570	0.976551	1.697976
B	0.805443	1.431603	-0.000618
B	-0.025434	-0.545259	2.129250
B	-0.025548	-0.544257	-2.129741
B	-0.493291	3.574306	0.000643
B	-0.332684	2.464440	1.142068
B	0.103760	-2.554115	-0.000712
B	0.957737	2.974907	0.000496

IrB₁₂⁻ (10, C_s)**-1 1**

Ir	0.000199	-0.001057	-1.450221
B	-0.000007	2.431748	2.650721
B	0.000090	-1.462081	4.234513
B	-0.000020	1.331647	3.824223
B	0.000009	-0.663162	1.469131
B	-0.000006	0.938222	1.949892
B	-0.000054	-2.259374	1.106750
B	-0.000010	-0.280823	3.127002
B	-0.000020	2.338402	1.110514
B	0.000005	-1.953387	2.670679
B	0.000051	-1.383596	-0.190681
B	-0.000018	0.010677	4.721570
B	0.000128	1.027048	0.135602