

Electronic Supporting Information

Analysis of the structures, stabilities and electronic properties of MB_{16}^- ($\text{M}=\text{V}, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}$) clusters and assembly

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Table S1 Cartesian coordinates for the low-lying isomers of MB_{16}^- (M=V, Cr, Mn, Fe, Co, Ni) clusters.

VB_{16}^-

1

-1 1

V	0.00000000	0.00000000	0.00041500
B	-1.50042300	1.44885900	-0.80895400
B	0.00000000	2.00593200	-0.83595800
B	-1.86462400	-0.79650200	0.82893900
B	1.86462400	0.79650200	0.82893900
B	-0.80038500	-2.00504800	0.77102000
B	1.86462400	-0.79650200	0.82893900
B	-1.50042300	-1.44885900	-0.80895400
B	2.19421100	0.00000000	-0.74700600
B	-1.86462400	0.79650200	0.82893900
B	0.80038500	2.00504800	0.77102000
B	0.00000000	-2.00593200	-0.83595800
B	1.50042300	-1.44885900	-0.80895400
B	-2.19421100	0.00000000	-0.74700600
B	1.50042300	1.44885900	-0.80895400
B	-0.80038500	2.00504800	0.77102000
B	0.80038500	-2.00504800	0.77102000

2

-1 3

V	0.00000000	0.00000000	0.00092900
B	-1.47203500	1.47203500	-0.80442900
B	1.94935600	-0.79258400	0.79029500
B	0.00000000	2.12300400	-0.77722900
B	0.79258400	-1.94935600	0.79029500
B	0.79258400	1.94935600	0.79029500
B	-2.12300400	0.00000000	-0.77722900
B	-0.79258400	-1.94935600	0.79029500
B	2.12300400	0.00000000	-0.77722900
B	0.00000000	-2.12300400	-0.77722900
B	1.47203500	-1.47203500	-0.80442900
B	-0.79258400	1.94935600	0.79029500
B	-1.94935600	0.79258400	0.79029500
B	1.94935600	0.79258400	0.79029500
B	-1.47203500	-1.47203500	-0.80442900
B	-1.94935600	-0.79258400	0.79029500
B	1.47203500	1.47203500	-0.80442900

3

-1 1

V	-0.00437700	-0.04420100	-0.50100400
B	-1.92560600	-0.45465900	0.62946400
B	-1.67039900	1.12939500	0.87986500
B	-0.24027100	1.83428700	1.09657300
B	-0.93964700	1.88262000	-0.45271600
B	-2.10424400	0.68579600	-0.74980200
B	-2.16558900	-0.83766300	-1.08514000
B	2.33120000	-0.33230500	-1.10770300
B	1.98143100	1.14533300	-0.67655800
B	2.11469000	-0.08446800	0.55705300
B	0.87862800	-0.90473200	1.33541300
B	0.27404300	-2.11785000	0.17313300
B	1.71432100	-1.54863900	-0.25567100
B	-1.28240000	-1.85582600	-0.27507700
B	-0.67553200	-1.27212400	1.31530500
B	1.04658000	0.87969200	1.24184900
B	0.68292900	2.05446500	-0.32137100

4

-1 1

V	0.00000000	0.00000000	0.51195900
B	-0.77474100	2.37408300	0.99632400
B	-0.89244800	0.81139100	-1.31414800
B	0.89244800	-0.81139100	-1.31414800
B	0.77474100	-2.37408300	0.99632400
B	0.00000000	1.94834700	-0.50801500
B	-2.06964700	0.00000000	-0.33485000
B	2.06964700	0.00000000	-0.33485000
B	0.00000000	-1.94834700	-0.50801500
B	0.77474100	2.37408300	0.99632400
B	-0.89244800	-0.81139100	-1.31414800
B	0.89244800	0.81139100	-1.31414800
B	-0.77474100	-2.37408300	0.99632400
B	-1.74354300	1.49740500	0.15050400
B	1.74354300	-1.49740500	0.15050400
B	1.74354300	1.49740500	0.15050400
B	-1.74354300	-1.49740500	0.15050400

CrB₁₆⁻

1

-1 2

Cr	0.00000000	0.00000000	0.01461300
B	0.00000000	2.10443800	-0.79027400
B	-2.10443800	0.00000000	-0.79027400
B	-1.45020700	-1.45020700	-0.83493800
B	0.00000000	-2.10443800	-0.79027400
B	1.45020700	-1.45020700	-0.83493800
B	1.45020700	1.45020700	-0.83493800
B	-0.78671000	1.93041900	0.80383800
B	-1.93041900	0.78671000	0.80383800
B	-0.78671000	-1.93041900	0.80383800
B	0.78671000	-1.93041900	0.80383800
B	1.93041900	-0.78671000	0.80383800
B	0.78671000	1.93041900	0.80383800
B	2.10443800	0.00000000	-0.79027400
B	1.93041900	0.78671000	0.80383800
B	-1.45020700	1.45020700	-0.83493800
B	-1.93041900	-0.78671000	0.80383800

2

-1 2

Cr	0.00095000	-0.02016800	-0.43213900
B	-2.25281200	-0.23453000	-1.15141400
B	-0.35383900	-2.15339200	0.15481200
B	2.06380600	-0.88754200	-1.11558500
B	2.08575400	0.62776900	-0.74138700
B	-0.57255600	2.12616000	-0.34176800
B	-2.10672500	-0.03060200	0.53369700
B	-0.91846400	-0.93151900	1.31697700
B	0.61705600	-1.33402100	1.29343200
B	1.68961000	1.05320900	0.88644900
B	0.29040200	1.79859100	1.10962500
B	-1.88044300	1.22050600	-0.65557800
B	-1.73164400	-1.49555900	-0.31995000
B	1.17740000	-1.91195400	-0.33030100
B	1.89321800	-0.54136700	0.61333200
B	1.01716800	1.90521300	-0.43487200
B	-1.02249200	0.88584200	1.25679800

3

-1 2

Cr	0.00060600	-0.28403000	0.00000000
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B	1.74180800	-0.38414200	1.46738300
B	-2.06885300	-0.45909200	-0.79246000
B	0.54270700	-1.12953300	-2.13855200
B	-0.94765100	-0.71374100	1.96095700
B	-1.13770700	0.99577400	1.39579300
B	1.74180800	-0.38414200	-1.46738300
B	-1.13770700	0.99577400	-1.39579300
B	1.31133300	1.21393400	0.79161500
B	1.31133300	1.21393400	-0.79161500
B	0.32896900	0.62003400	1.97390400
B	0.32896900	0.62003400	-1.97390400
B	2.29536200	-0.00781100	0.00000000
B	-1.83948200	1.08468900	0.00000000
B	0.54270700	-1.12953300	2.13855200
B	-0.94765100	-0.71374100	-1.96095700
B	-2.06885300	-0.45909200	0.79246000

4

-1 2

Cr	0.16775800	-0.18190100	0.00000000
B	-1.80691500	0.39919800	0.80602900
B	1.86592100	-0.34656200	1.47732700
B	-1.65950600	-1.28424000	0.00000000
B	-0.21820400	1.70316800	0.80030800
B	-0.21820400	1.70316800	-0.80030800
B	-1.09312500	-1.12956200	-1.48258400
B	2.38826000	-0.49874500	0.00000000
B	-1.80691500	0.39919800	-0.80602900
B	0.38125300	-0.72503300	-2.11768700
B	0.84783900	0.90834200	-1.82399300
B	1.86592100	-0.34656200	-1.47732700
B	-0.74376500	0.51850300	-1.97895400
B	0.38125300	-0.72503300	2.11768700
B	-0.74376500	0.51850300	1.97895400
B	-1.09312500	-1.12956200	1.48258400
B	0.84783900	0.90834200	1.82399300

MnB₁₆⁻

1

-1 3

Mn	0.00000000	0.00000000	0.00067100
B	-0.78409000	1.92349700	0.81071100
B	1.92349700	0.78409000	0.81071100

B	1.92349700	-0.78409000	0.81071100
B	0.78409000	-1.92349700	0.81071100
B	-0.78409000	-1.92349700	0.81071100
B	-1.92349700	0.78409000	0.81071100
B	0.00000000	2.09513900	-0.78922900
B	1.45048300	1.45048300	-0.83303200
B	1.45048300	-1.45048300	-0.83303200
B	0.00000000	-2.09513900	-0.78922900
B	-1.45048300	-1.45048300	-0.83303200
B	-1.45048300	1.45048300	-0.83303200
B	-1.92349700	-0.78409000	0.81071100
B	-2.09513900	0.00000000	-0.78922900
B	0.78409000	1.92349700	0.81071100
B	2.09513900	0.00000000	-0.78922900

2

-1 3

Mn	-0.00603900	-0.20672300	0.00000000
B	1.35259700	1.20149500	0.79570800
B	1.35259700	1.20149500	-0.79570800
B	-1.14892500	0.98933600	-1.41491600
B	-1.83091800	1.08899000	0.00000000
B	-1.14892500	0.98933600	1.41491600
B	0.32824200	0.61214900	1.95332700
B	2.29490000	-0.02936000	0.00000000
B	0.32824200	0.61214900	-1.95332700
B	-0.94836900	-0.76295400	-1.93599500
B	-2.06531500	-0.46176300	0.79041700
B	-0.94836900	-0.76295400	1.93599500
B	0.53428900	-1.18255000	2.10407600
B	1.73058700	-0.40872200	1.46313900
B	1.73058700	-0.40872200	-1.46313900
B	0.53428900	-1.18255000	-2.10407600
B	-2.06531500	-0.46176300	-0.79041700

3

-1 3

Mn	0.01260000	-0.01204000	-0.38610100
B	0.62407800	-1.36152600	1.28050800
B	1.88653500	-0.53771000	0.60077400
B	-0.93204300	-0.98634200	1.31644800
B	1.66997900	1.04783400	0.89491400
B	-0.58553900	2.09587300	-0.36600800
B	-2.33946700	-0.23877300	-1.14080400
B	-1.89608200	1.21312000	-0.76677900
B	0.26756500	1.79466500	1.12902400

B	-0.99244700	0.83210600	1.36243500
B	2.10323900	-0.86353200	-1.14298100
B	1.19325400	-1.88995900	-0.38814500
B	1.00746000	1.90379300	-0.42565400
B	-2.06950500	0.00580600	0.53346900
B	-0.34232900	-2.12542400	0.10257500
B	2.09879600	0.64600500	-0.74915900
B	-1.75649100	-1.47573900	-0.31011200

4

-1 3

Mn	-0.01296100	0.13217800	-0.14870400
B	0.84312400	-0.19978500	1.72936100
B	-1.48516100	-1.06672000	-1.11816300
B	0.07507700	2.29592800	-0.65408300
B	-2.12680100	0.41677200	-0.72067500
B	1.46187600	-1.20186900	-1.07772000
B	1.81369000	0.86866200	0.82880800
B	0.68425900	-1.73889400	0.58723800
B	1.93711600	-0.75080700	0.55185600
B	-0.67938900	0.25875100	1.84227900
B	2.10095300	0.27533700	-0.80728400
B	-1.94060200	-0.71388200	0.53992600
B	-0.03252100	-1.72819000	-1.23701100
B	-1.42873200	1.83845500	-0.46509400
B	-0.90476700	-1.90673000	0.31850000
B	1.55448000	1.80132100	-0.49438000
B	-1.80779600	0.89076100	0.91996200

FeB₁₆⁻

1

-1 4

Fe	0.00000000	0.00000000	0.00000000
B	0.00000000	2.08351500	0.80419000
B	-1.92491700	-0.79732700	-0.80419000
B	0.79732700	1.92491700	-0.80419000
B	-1.47326700	-1.47326700	0.80419000
B	1.47326700	1.47326700	0.80419000
B	-0.79732700	-1.92491700	-0.80419000
B	1.92491700	0.79732700	-0.80419000
B	0.00000000	-2.08351500	0.80419000
B	0.79732700	-1.92491700	-0.80419000
B	2.08351500	0.00000000	0.80419000
B	1.47326700	-1.47326700	0.80419000
B	1.92491700	-0.79732700	-0.80419000

B	-1.92491700	0.79732700	-0.80419000
B	-1.47326700	1.47326700	0.80419000
B	-2.08351500	0.00000000	0.80419000
B	-0.79732700	1.92491700	-0.80419000

2

-1 2

Fe	-0.02054800	0.09247900	-0.16689800
B	-1.95375300	-0.61038700	0.60315100
B	2.03126200	0.08696300	-0.94837800
B	1.61894800	1.65657400	-0.71507800
B	1.83230800	0.84523100	0.68824200
B	1.88570200	-0.82154200	0.51476700
B	1.30953500	-1.37930100	-0.99801600
B	0.16993100	2.24171200	-0.75613200
B	-1.64703500	1.00588100	0.97628400
B	0.56581300	-1.63183200	0.88890900
B	-1.61368000	-1.08233700	-1.04624900
B	-2.09459100	0.51586200	-0.65368300
B	-0.96994800	-1.84522700	0.37501100
B	-0.42774800	0.54599300	1.88549600
B	0.98961100	-0.12904900	1.77762400
B	-0.24237100	-1.78096200	-1.28140200
B	-1.34713600	1.90152700	-0.44267600

3

-1 4

Fe	0.00000000	0.00000000	0.97305200
B	0.81412700	1.96547700	-1.06153400
B	1.96547700	-0.81412700	-1.06153400
B	0.00000000	2.11026300	0.42905100
B	1.49218100	-1.49218100	0.42905100
B	-1.96547700	-0.81412700	-1.06153400
B	-1.49218100	-1.49218100	0.42905100
B	-1.49218100	1.49218100	0.42905100
B	0.00000000	-2.11026300	0.42905100
B	-0.81412700	1.96547700	-1.06153400
B	0.81412700	-1.96547700	-1.06153400
B	-1.96547700	0.81412700	-1.06153400
B	-0.81412700	-1.96547700	-1.06153400
B	1.49218100	1.49218100	0.42905100
B	2.11026300	0.00000000	0.42905100
B	-2.11026300	0.00000000	0.42905100
B	1.96547700	0.81412700	-1.06153400

4

-1 2

Fe	0.00000000	0.00000000	0.00000000
B	-0.51217400	-1.36157000	1.61970900
B	0.51217400	1.36157000	1.61970900
B	1.36157000	-0.51217400	-1.61970900
B	-1.36157000	0.51217400	-1.61970900
B	-0.43509500	1.88721600	-1.13992200
B	0.43509500	-1.88721600	-1.13992200
B	0.00000000	2.14711300	0.34987300
B	0.00000000	-2.14711300	0.34987300
B	2.14711300	0.00000000	-0.34987300
B	-2.14711300	0.00000000	-0.34987300
B	-1.88721600	-0.43509500	1.13992200
B	1.88721600	0.43509500	1.13992200
B	-0.31679400	-0.78247600	-1.99995900
B	0.31679400	0.78247600	-1.99995900
B	0.78247600	-0.31679400	1.99995900
B	-0.78247600	0.31679400	1.99995900

CoB₁₆⁻

1

-1 3

Co	0.00000000	0.00000000	0.00000000
B	0.00000000	2.07433600	0.80928100
B	0.79381400	-1.91643700	-0.80928100
B	-0.79381400	1.91643700	-0.80928100
B	0.00000000	-2.07433600	0.80928100
B	-1.91643700	-0.79381400	-0.80928100
B	2.07433600	0.00000000	0.80928100
B	1.46677700	1.46677700	0.80928100
B	-0.79381400	-1.91643700	-0.80928100
B	-2.07433600	0.00000000	0.80928100
B	1.91643700	0.79381400	-0.80928100
B	-1.46677700	-1.46677700	0.80928100
B	0.79381400	1.91643700	-0.80928100
B	1.91643700	-0.79381400	-0.80928100
B	-1.46677700	1.46677700	0.80928100
B	1.46677700	-1.46677700	0.80928100
B	-1.91643700	0.79381400	-0.80928100

2

-1 1

Co	0.00000000	0.00000000	0.00000000
B	1.09414300	-1.60735600	1.15336900
B	-0.76233800	1.98141400	-0.33623500
B	0.76233800	-1.98141400	-0.33623500

B	-1.09414300	1.60735600	1.15336900
B	0.00000000	-1.45791100	-1.61465100
B	-1.45791100	0.00000000	1.61465100
B	1.45791100	0.00000000	1.61465100
B	0.00000000	1.45791100	-1.61465100
B	1.60735600	1.09414300	-1.15336900
B	1.98141400	0.76233800	0.33623500
B	-1.98141400	-0.76233800	0.33623500
B	-1.60735600	-1.09414300	-1.15336900
B	-0.84929600	0.02756600	-1.98263900
B	-0.02756600	-0.84929600	1.98263900
B	0.02756600	0.84929600	1.98263900
B	0.84929600	-0.02756600	-1.98263900

3

-1 1

Co	0.03070800	0.01431900	-0.20937200
B	-2.02138400	0.13327000	0.46456900
B	-0.94963200	0.75041600	1.48340100
B	0.30532800	1.70801500	1.15300600
B	-0.43555000	2.15074800	-0.43916700
B	-1.76237700	1.31740800	-0.86411800
B	1.66628000	0.90986500	0.89650500
B	-1.00206800	-1.01073100	1.26417000
B	0.54849700	-1.43370300	1.20765800
B	-1.79129300	-1.36199400	-0.40213800
B	2.05342900	0.58277000	-0.79176500
B	1.85035100	-0.66756500	0.53248400
B	-0.45857800	-2.14306600	0.04562400
B	1.11029300	1.90961600	-0.39480700
B	-2.26953300	-0.09883900	-1.23762100
B	1.94807300	-0.89571900	-1.25828600
B	1.04234000	-1.92781400	-0.52890800

4

-1 1

Co	0.01929600	0.07446200	-0.10477700
B	-0.50314600	-1.65421700	0.91030000
B	-2.01724000	0.02216100	-0.98876500
B	-0.26560700	2.17304300	-0.80373100
B	1.26675000	1.93258100	-0.48096500
B	0.40674800	0.59605500	1.87533600
B	-0.98207100	-0.14750800	1.77605700
B	1.61190200	1.08259900	0.95773200
B	1.66121400	-1.02325800	-1.06340600
B	-1.71897400	1.60029600	-0.73575100

B	-1.24345800	-1.39921600	-1.03367100
B	2.05893700	0.58036800	-0.69553200
B	-1.83734400	-0.88148000	0.50905700
B	1.95940400	-0.52795600	0.60148600
B	1.03081300	-1.80001200	0.37342400
B	-1.84717000	0.79146300	0.68057200
B	0.31504500	-1.74701500	-1.31634800

NiB₁₆⁻

1

-1 2

Ni	0.84276600	-0.55788800	0.00000000
B	-0.81192300	1.61845000	1.94694600
B	-1.22448000	0.13212400	0.80151700
B	-1.06044800	-1.37871200	0.00000000
B	-1.22448000	0.13212400	-0.80151700
B	-0.81192300	1.61845000	-1.94694600
B	0.60481100	0.90370000	1.38180500
B	-0.43880300	-1.28134400	1.74021100
B	-0.01843500	-2.48345700	-0.76976800
B	-0.57815100	0.16401000	-2.44732300
B	1.21627800	1.52951100	0.00000000
B	0.60481100	0.90370000	-1.38180500
B	0.02932200	2.43320400	-0.80963800
B	-0.57815100	0.16401000	2.44732300
B	-0.01843500	-2.48345700	0.76976800
B	-0.43880300	-1.28134400	-1.74021100
B	0.02932200	2.43320400	0.80963800

2

-1 2

Ni	-0.11441700	-0.55959000	-0.97610000
B	1.04313800	0.07394200	1.19393300
B	1.82523200	0.20676200	-0.51489400
B	-2.30280800	-0.68767700	1.08154100
B	-1.81016200	0.30574200	-0.23159400
B	-0.37680200	-0.76573800	1.10368000
B	2.57729000	0.87275000	1.00620200
B	0.70749700	1.25525600	-1.01421100
B	1.42432500	1.83299800	0.50867300
B	2.63070800	-0.65592700	0.73851300
B	-2.43697700	0.84735300	1.22541500
B	-1.46724400	-1.91976900	0.51104000
B	1.44341400	-1.59095600	0.25622700
B	-0.07217600	2.32089500	0.08889800

B	0.00363800	-2.27914900	0.21986700
B	-1.64733300	1.93633300	0.33779000
B	-0.90100400	1.38089000	-1.04491700
3			
-1 2			
Ni	0.44404600	-0.98394500	0.00000000
B	-2.50741900	0.11337100	0.00000000
B	-1.84635700	0.58477800	1.42376600
B	1.88919200	0.20183600	1.55418300
B	-0.34477800	-0.34530400	-1.80500300
B	-0.34477800	-0.34530400	1.80500300
B	-1.44019000	-0.96003800	0.79721300
B	0.79665300	0.78548200	-2.51777700
B	-0.67573500	1.25744000	-2.27259700
B	1.88919200	0.20183600	-1.55418300
B	2.15175700	0.16747800	0.00000000
B	0.55571600	1.09042500	-0.81571000
B	0.55571600	1.09042500	0.81571000
B	0.79665300	0.78548200	2.51777700
B	-0.67573500	1.25744000	2.27259700
B	-1.84635700	0.58477800	-1.42376600
B	-1.44019000	-0.96003800	-0.79721300
4			
-1 2			
Ni	0.00000000	0.00000000	1.12818900
B	0.00000000	1.91503300	-0.06209100
B	0.00000000	-1.91503300	-0.06209100
B	-1.31408200	-0.85218500	-0.38983500
B	1.31408200	0.85218500	-0.38983500
B	-2.04377700	-0.37637400	1.01986300
B	-1.09872700	0.18458700	-1.71759500
B	1.72160200	-0.79457500	-0.06785200
B	2.04377700	0.37637400	1.01986300
B	1.09872700	-0.18458700	-1.71759500
B	-1.72160200	0.79457500	-0.06785200
B	0.33450100	1.24169000	-1.71494600
B	1.19706100	1.70941100	1.02953000
B	-1.17665600	1.81724000	-1.25600100
B	-0.33450100	-1.24169000	-1.71494600
B	-1.19706100	-1.70941100	1.02953000
B	1.17665600	-1.81724000	-1.25600100

Table S2 Bond length and dihedral angle for the stable isomers of MB₁₆⁻ (M=V, Cr, Mn, Fe, Co, Ni)

clusters.

VB₁₆⁻

R(1-3)	2.173	A(1-7-9)	70.3
R(1-7)	2.19	A(1-7-17)	72.4
R(1-10)	2.19	A(10-1-12)	118.8
R(1-12)	2.173	A(1-10-4)	68.7
R(2-3)	1.601	A(1-10-14)	70.3
R(2-14)	1.608	A(1-10-16)	72.4
R(3-15)	1.601	A(1-12-8)	70.9
R(3-16)	1.795	A(1-12-13)	70.9
R(4-6)	1.611	A(1-12-17)	69.8
R(4-8)	1.8	A(3-2-14)	136
R(4-10)	1.593	A(2-3-15)	139.2
R(5-7)	1.593	A(2-3-16)	64.3
R(5-11)	1.611	A(2-14-8)	128.6
R(5-15)	1.8	A(2-14-10)	63.6
R(6-17)	1.601	A(15-3-16)	113.7
R(7-9)	1.796	A(3-15-5)	109.3
R(7-17)	1.611	A(3-15-9)	136
R(8-12)	1.601	A(3-16-10)	109.1
R(8-14)	1.608	A(3-16-11)	63.5
R(9-13)	1.608	A(6-4-8)	64
R(9-15)	1.608	A(6-4-10)	138.6
R(10-14)	1.796	A(4-6-17)	131.3
R(10-16)	1.611	A(8-4-10)	111.2
R(11-16)	1.601	A(4-8-12)	109.3
R(12-13)	1.601	A(4-8-14)	63.3
R(12-17)	1.795	A(4-10-14)	63.7
A(3-1-7)	118.8	A(4-10-16)	138.6
A(3-1-10)	79	A(7-5-11)	138.6
A(3-1-12)	134.7	A(7-5-15)	111.2
A(1-3-2)	70.9	A(5-7-9)	63.7
A(1-3-15)	70.9	A(5-7-17)	138.6
A(1-3-16)	69.8	A(11-5-15)	64
A(7-1-10)	135.5	A(5-11-16)	131.3
A(7-1-12)	79	A(5-15-9)	63.3
A(1-7-5)	68.7	A(6-17-7)	131.3
A(6-17-12)	63.5	A(8-12-17)	113.7
A(9-7-17)	115	A(8-14-10)	110.7

A(7-9-13)	63.6	A(13-9-15)	128.6
A(7-9-15)	110.7	A(9-13-12)	136
A(7-17-12)	109.1	A(14-10-16)	115
A(12-8-14)	136	A(10-16-11)	131.3
A(8-12-13)	139.2	A(13-12-17)	64.3

CrB₁₆⁻

R(1-4)	2.22	A(1-16-9)	65.9
R(1-6)	2.22	A(7-2-13)	65.4
R(1-7)	2.22	A(7-2-16)	131.3
R(1-16)	2.22	A(2-7-14)	138.4
R(2-7)	1.592	A(13-2-16)	112.7
R(2-13)	1.786	A(2-13-8)	63.9
R(2-16)	1.592	A(2-13-15)	112.4
R(3-4)	1.592	A(2-16-3)	138.4
R(3-16)	1.592	A(2-16-9)	111.3
R(3-17)	1.786	A(4-3-16)	131.3
R(4-5)	1.592	A(4-3-17)	65.4
R(5-6)	1.592	A(3-4-5)	138.4
R(5-11)	1.786	A(16-3-17)	112.7
R(6-12)	1.832	A(3-16-9)	62.4
R(6-14)	1.592	A(3-17-9)	63.9
R(7-14)	1.592	A(3-17-10)	112.4
R(8-9)	1.617	A(4-5-6)	131.3
R(8-13)	1.573	A(4-5-11)	112.7
R(9-16)	1.832	A(6-5-11)	65.4
R(9-17)	1.573	A(5-6-12)	111.3
R(10-11)	1.573	A(5-6-14)	138.4
R(10-17)	1.617	A(5-11-10)	63.9
R(11-12)	1.617	A(5-11-12)	112.4
R(12-15)	1.573	A(12-6-14)	62.4
R(13-15)	1.617	A(6-12-11)	63.8
R(14-15)	1.786	A(6-12-15)	111.2
A(4-1-6)	81.6	A(6-14-7)	131.3
A(4-1-7)	135	A(6-14-15)	112.7
A(4-1-16)	81.6	A(7-14-15)	65.4
A(1-4-3)	70.3	A(9-8-13)	135
A(1-4-5)	70.3	A(8-9-16)	63.8
A(6-1-7)	81.6	A(8-9-17)	135
A(6-1-16)	135	A(8-13-15)	135
A(1-6-5)	70.3	A(16-9-17)	111.2
A(1-6-12)	65.9	A(9-17-10)	135
A(1-6-14)	70.3	A(11-10-17)	135

A(7-1-16)	81.6	A(10-11-12)	135
A(1-7-2)	70.3	A(11-12-15)	135
A(1-7-14)	70.3	A(12-15-13)	135
A(1-16-2)	70.3	A(12-15-14)	63.9
A(1-16-3)	70.3	A(13-15-14)	112.4

MnB₁₆⁻

R(1-9)	2.214	A(7-2-8)	112.2
R(1-10)	2.214	A(7-2-16)	135
R(1-12)	2.214	A(2-7-13)	64
R(1-13)	2.214	A(2-7-14)	135
R(2-7)	1.611	A(8-2-16)	64
R(2-8)	1.79	A(2-8-9)	112.7
R(2-16)	1.568	A(2-8-13)	65.5
R(3-4)	1.568	A(2-16-3)	135
R(3-16)	1.611	A(2-16-9)	111.3
R(4-5)	1.611	A(4-3-16)	135
R(4-17)	1.79	A(3-4-5)	135
R(5-6)	1.568	A(3-4-17)	64
R(5-10)	1.836	A(3-16-9)	64
R(6-11)	1.79	A(5-4-17)	112.2
R(6-14)	1.611	A(4-5-6)	135
R(7-13)	1.836	A(4-5-10)	64
R(7-14)	1.568	A(4-17-9)	112.7
R(8-9)	1.588	A(4-17-10)	65.5
R(8-13)	1.588	A(6-5-10)	111.3
R(9-16)	1.836	A(5-6-11)	64
R(9-17)	1.588	A(5-6-14)	135
R(10-11)	1.588	A(5-10-11)	62.6
R(10-17)	1.588	A(5-10-17)	111
R(11-12)	1.588	A(11-6-14)	112.2
R(12-15)	1.588	A(6-11-10)	112.7
R(13-15)	1.588	A(6-11-12)	65.5
R(14-15)	1.79	A(6-14-7)	135
A(9-1-10)	81.8	A(6-14-15)	112.2
A(9-1-12)	135.8	A(13-7-14)	111.3
A(9-1-13)	81.8	A(7-13-8)	111
A(1-9-8)	70	A(7-13-15)	62.6
A(1-9-16)	66	A(7-14-15)	64
A(1-9-17)	70	A(9-8-13)	132
A(10-1-12)	81.8	A(8-9-16)	62.6
A(10-1-13)	135.8	A(8-9-17)	137.8
A(1-10-5)	66	A(8-13-15)	137.8

A(1-10-11)	70	A(16-9-17)	111
A(1-10-17)	70	A(9-17-10)	132
A(12-1-13)	81.8	A(11-10-17)	137.8
A(1-12-11)	70	A(10-11-12)	132
A(1-12-15)	70	A(11-12-15)	137.8
A(1-13-7)	66	A(12-15-13)	132
A(1-13-8)	70	A(12-15-14)	65.5
A(1-13-15)	70	A(13-15-14)	112.7

FeB₁₆⁻

R(1-6)	2.233	A(1-16-5)	69.1
R(1-7)	2.233	A(1-16-14)	66.2
R(1-12)	2.233	A(1-16-15)	69.1
R(1-16)	2.233	A(1-17-4)	69.1
R(1-17)	2.233	A(1-17-14)	69.1
R(2-6)	1.595	A(1-17-15)	66.2
R(2-15)	1.595	A(6-2-15)	135
R(3-7)	1.595	A(2-6-8)	112
R(3-14)	1.595	A(2-6-11)	135
R(4-8)	1.595	A(2-15-16)	135
R(4-17)	1.595	A(2-15-17)	63.7
R(5-7)	1.802	A(7-3-14)	135
R(5-9)	1.595	A(3-7-5)	63.7
R(5-16)	1.595	A(3-7-10)	135
R(6-8)	1.802	A(3-14-16)	63.7
R(6-11)	1.595	A(3-14-17)	135
R(7-10)	1.595	A(8-4-17)	135
R(8-13)	1.595	A(4-8-6)	63.7
R(9-10)	1.802	A(4-8-13)	135
R(9-12)	1.595	A(4-17-14)	135
R(10-13)	1.595	A(4-17-15)	112
R(11-12)	1.595	A(7-5-9)	63.7
R(12-13)	1.802	A(7-5-16)	112
R(14-16)	1.802	A(5-7-10)	112
R(14-17)	1.595	A(9-5-16)	135
R(15-16)	1.595	A(5-9-10)	112
R(15-17)	1.802	A(5-9-12)	135
A(6-1-7)	159	A(5-16-14)	112
A(6-1-12)	82.5	A(5-16-15)	135
A(6-1-16)	119.1	A(8-6-11)	63.7
A(6-1-17)	78.3	A(6-8-13)	112
A(1-6-2)	69.1	A(6-11-12)	135
A(1-6-8)	66.2	A(7-10-9)	63.7

A(1-6-11)	69.1	A(7-10-13)	135
A(7-1-12)	78.3	A(8-13-10)	135
A(7-1-16)	78.3	A(8-13-12)	112
A(7-1-17)	119.1	A(10-9-12)	63.7
A(1-7-3)	69.1	A(9-10-13)	112
A(1-7-5)	66.2	A(9-12-11)	135
A(1-7-10)	69.1	A(9-12-13)	112
A(12-1-16)	119.1	A(10-13-12)	63.7
A(12-1-17)	159	A(11-12-13)	63.7
A(1-12-9)	69.1	A(16-14-17)	112
A(1-12-11)	69.1	A(14-16-15)	63.7
A(1-12-13)	66.2	A(14-17-15)	63.7
A(16-1-17)	78.3	A(16-15-17)	112

CoB₁₆⁻

R(1-8)	2.227	A(4-2-15)	64
R(1-12)	2.227	A(2-4-13)	64
R(1-15)	2.227	A(2-4-17)	111.8
R(1-16)	2.227	A(8-2-15)	135
R(2-4)	1.81	A(2-8-7)	135
R(2-8)	1.588	A(2-8-13)	64
R(2-15)	1.588	A(2-15-10)	135
R(3-5)	1.81	A(2-15-17)	111.8
R(3-9)	1.588	A(5-3-9)	64
R(3-14)	1.588	A(5-3-14)	111.8
R(4-13)	1.588	A(3-5-12)	111.8
R(4-17)	1.588	A(3-5-16)	64
R(5-12)	1.588	A(9-3-14)	135
R(5-16)	1.588	A(3-9-6)	135
R(6-9)	1.588	A(3-9-12)	111.8
R(6-10)	1.81	A(3-14-11)	135
R(6-17)	1.588	A(3-14-16)	64
R(7-8)	1.588	A(13-4-17)	135
R(7-11)	1.81	A(4-13-8)	111.8
R(7-16)	1.588	A(4-13-11)	135
R(8-13)	1.81	A(4-17-6)	135
R(9-12)	1.81	A(4-17-15)	64
R(10-12)	1.588	A(12-5-16)	135
R(10-15)	1.588	A(5-12-9)	64
R(11-13)	1.588	A(5-12-10)	135
R(11-14)	1.588	A(5-16-7)	135
R(14-16)	1.81	A(5-16-14)	111.8
R(15-17)	1.81	A(9-6-10)	111.8

A(8-1-12)	137.4	A(9-6-17)	135
A(8-1-15)	82.4	A(6-9-12)	64
A(8-1-16)	82.4	A(10-6-17)	64
A(1-8-2)	69.1	A(6-10-12)	64
A(1-8-7)	69.1	A(6-10-15)	111.8
A(1-8-13)	66	A(6-17-15)	111.8
A(12-1-15)	82.4	A(8-7-11)	64
A(12-1-16)	82.4	A(8-7-16)	135
A(1-12-5)	69.1	A(7-8-13)	111.8
A(1-12-9)	66	A(11-7-16)	111.8
A(1-12-10)	69.1	A(7-11-13)	111.8
A(15-1-16)	137.4	A(7-11-14)	64
A(1-15-2)	69.1	A(7-16-14)	64
A(1-15-10)	69.1	A(8-13-11)	64
A(1-15-17)	66	A(9-12-10)	111.8
A(1-16-5)	69.1	A(12-10-15)	135
A(1-16-7)	69.1	A(10-15-17)	64
A(1-16-14)	66	A(13-11-14)	135
A(4-2-8)	111.8	A(11-14-16)	111.8

NiB₁₆⁻

R(1-7)	2.025	A(3-2-7)	69.7
R(1-12)	2.025	A(3-2-14)	60.1
R(1-15)	2.245	A(3-2-17)	94.7
R(1-16)	2.279	A(2-3-5)	126.6
R(2-3)	1.921	A(2-3-8)	101.3
R(2-7)	1.684	A(7-2-14)	65.5
R(2-14)	1.556	A(7-2-17)	62.9
R(2-17)	1.632	A(2-7-11)	115.8
R(3-5)	1.603	A(14-2-17)	127.8
R(3-8)	1.87	A(2-14-8)	135.1
R(4-5)	1.718	A(2-17-11)	115.3
R(4-15)	1.703	A(2-17-13)	134.2
R(5-6)	1.921	A(5-3-8)	120.1
R(5-16)	1.87	A(3-5-4)	62.2
R(6-10)	1.556	A(3-5-6)	126.6
R(6-12)	1.684	A(3-5-16)	120.1
R(6-13)	1.632	A(3-8-14)	60.5
R(7-11)	1.636	A(3-8-15)	111.9
R(8-14)	1.615	A(5-4-15)	147.1
R(8-15)	1.601	A(4-5-6)	159.7
R(9-15)	1.54	A(4-5-16)	61.9

R(9-16)	1.601	A(4-15-8)	68
R(10-16)	1.615	A(4-15-9)	63.1
R(11-12)	1.636	A(6-5-16)	101.3
R(11-17)	1.697	A(5-6-10)	60.1
R(13-17)	1.619	A(5-6-12)	69.7
A(7-1-12)	86	A(5-6-13)	94.7
A(7-1-15)	109.9	A(5-16-9)	111.9
A(7-1-16)	133.2	A(5-16-10)	60.5
A(1-7-2)	129.3	A(10-6-12)	65.5
A(1-7-11)	69.9	A(10-6-13)	127.8
A(12-1-15)	143.9	A(6-10-16)	135.1
A(12-1-16)	69	A(12-6-13)	62.9
A(1-12-6)	129.3	A(6-12-11)	115.8
A(1-12-11)	69.9	A(6-13-17)	134.2
A(15-1-16)	76.9	A(7-11-12)	115.3
A(1-15-4)	61.5	A(7-11-17)	62.6
A(1-15-8)	70.4	A(14-8-15)	163.7
A(1-15-9)	70	A(8-15-9)	127.3
A(1-16-5)	67.2	A(15-9-16)	127.3
A(1-16-9)	68.2	A(9-16-10)	163.7
A(1-16-10)	95.7	A(12-11-17)	110.2
		A(11-17-13)	61.5

Table S3 The local magnetic moment (μ_s) and total magnetic moment ($\Sigma\mu_s$) of the M and B atoms of MB_{16}^- (M=V, Cr, Mn, Fe, Co, Ni) clusters for the lowest energy structures.

$VB_{16}^- (2\mu_B)$		$CrB_{16}^- (1\mu_B)$		$MnB_{16}^- (2\mu_B)$		$FeB_{16}^- (3\mu_B)$		$CoB_{16}^- (2\mu_B)$		$NiB_{16}^- (1\mu_B)$	
V(μ_s)	B(μ_s)	Cr(μ_s)	B(μ_s)	Mn(μ_s)	B(μ_s)	Fe(μ_s)	B(μ_s)	Co(μ_s)	B(μ_s)	Ni(μ_s)	B(μ_s)
0.089	-0.038	-1.228	0.014	-1.445	-0.031	-1.504	-0.094	-0.243	-0.113	-0.467	0.003
	-0.133		0.014		-0.031		-0.094		-0.109		-0.112
	-0.220		0.015		-0.031		-0.094		-0.112		-0.017
	-0.133		0.014		-0.024		-0.093		-0.114		-0.112
	-0.132		0.015		-0.042		-0.094		-0.126		0.003
	-0.219		0.015		-0.031		-0.094		-0.109		-0.035
	-0.130		0.014		0.072		-0.094		-0.110		0.013
	-0.038		0.014		-0.145		-0.092		-0.113		-0.067
	-0.133		0.014		-0.147		-0.094		-0.058		0.000
	-0.220		0.014		0.071		-0.094		-0.110		0.055
	-0.133		0.014		-0.147		-0.093		-0.120		-0.035
	-0.038		0.014		-0.147		-0.094		-0.109		-0.088
	-0.219		0.014		-0.033		-0.094		-0.107		0.000
	-0.133		0.014		0.070		-0.094		-0.120		-0.067
	-0.038		0.015		-0.030		-0.094		-0.111		0.013
	-0.133		0.014		0.071		-0.090		-0.126		-0.088

Table S4 Cartesian coordinates for the stable isomers of $\text{Fe}_2\text{B}_{24}^-$ and $\text{Co}_2\text{B}_{24}^-$ clusters. $\text{Fe}_2\text{B}_{24}^-$

-1 6

B	-1.96396100	-0.81092500	-1.75645100
B	1.96396100	0.81092500	-1.75645100
B	-0.81092500	-1.96396100	-1.75645100
B	1.96396100	-0.81092500	-1.75645100
B	-1.96396100	0.81092500	-1.75645100
B	0.81092500	1.96396100	-1.75645100
B	-0.81092500	1.96396100	-1.75645100
B	0.81092500	-1.96396100	-1.75645100
Fe	0.00000000	0.00000000	1.84484500
B	-1.46702300	1.46702300	-0.15306200
B	0.00000000	2.21592900	-0.15049800
B	-1.96676400	-0.81250700	1.44524000
B	1.96676400	0.81250700	1.44524000
B	-0.81250700	-1.96676400	1.44524000
B	1.96676400	-0.81250700	1.44524000
B	-1.46702300	-1.46702300	-0.15306200
B	2.21592900	0.00000000	-0.15049800
B	-1.96676400	0.81250700	1.44524000
B	0.81250700	1.96676400	1.44524000
B	0.00000000	-2.21592900	-0.15049800
B	1.46702300	-1.46702300	-0.15306200
B	-2.21592900	0.00000000	-0.15049800
B	1.46702300	1.46702300	-0.15306200
B	-0.81250700	1.96676400	1.44524000
B	0.81250700	-1.96676400	1.44524000
Fe	0.00000000	0.00000000	-1.13255200

 $\text{Co}_2\text{B}_{24}^-$

-1 2

Co	0.00000000	0.00000000	-1.06068800
B	0.80433400	-1.95029900	-1.71013900
B	0.00000000	2.23379800	-0.12710200
B	0.00000000	-2.23379800	-0.12710200
B	-0.80433400	1.95029900	-1.71013900
B	-2.23379800	0.00000000	-0.12710200
B	1.95029900	0.80433400	-1.71013900
B	1.95029900	-0.80433400	-1.71013900
B	-1.45420400	1.45420400	-0.12751800
B	-1.95029900	-0.80433400	-1.71013900

B	2.23379800	0.00000000	-0.12710200
B	-1.95029900	0.80433400	-1.71013900
B	1.45420400	-1.45420400	-0.12751800
B	1.45420400	1.45420400	-0.12751800
B	-0.80433400	-1.95029900	-1.71013900
B	0.80433400	1.95029900	-1.71013900
B	-1.45420400	-1.45420400	-0.12751800
B	0.80964900	-1.95732100	1.46115000
B	-0.80964900	1.95732100	1.46115000
B	1.95732100	0.80964900	1.46115000
B	1.95732100	-0.80964900	1.46115000
B	-1.95732100	-0.80964900	1.46115000
B	-1.95732100	0.80964900	1.46115000
B	-0.80964900	-1.95732100	1.46115000
B	0.80964900	1.95732100	1.46115000
Co	0.00000000	0.00000000	1.61816700

Table S5 Bond length and dihedral angle for the stable isomers of $\text{Fe}_2\text{B}_{24}^-$ and $\text{Co}_2\text{B}_{24}^-$ clusters. $\text{Fe}_2\text{B}_{24}^-$

R(1-3)	1.631	A(14-9-18)	88
R(1-5)	1.622	A(14-9-19)	158.7
R(2-4)	1.622	A(9-14-12)	67.9
R(2-6)	1.631	A(9-14-16)	92.8
R(3-8)	1.622	A(9-14-25)	68
R(3-16)	1.802	A(15-9-18)	158.7
R(3-26)	2.214	A(15-9-19)	88
R(4-8)	1.631	A(9-15-13)	68
R(4-17)	1.817	A(9-15-17)	96.9
R(4-26)	2.214	A(9-15-25)	67.9
R(5-7)	1.631	A(18-9-19)	88
R(5-22)	1.817	A(9-18-12)	68
R(5-26)	2.214	A(9-18-22)	96.9
R(6-7)	1.622	A(9-18-24)	67.9
R(6-23)	1.802	A(9-19-13)	67.9
R(6-26)	2.214	A(9-19-23)	92.8
R(7-10)	1.802	A(9-19-24)	68
R(8-21)	1.802	A(11-10-22)	144.1
R(9-14)	2.165	A(11-10-24)	63.1
R(9-15)	2.165	A(10-11-23)	125.9
R(9-18)	2.165	A(22-10-24)	114.3
R(9-19)	2.165	A(10-22-16)	125.9
R(10-11)	1.647	A(10-22-18)	62.5
R(10-22)	1.647	A(10-24-18)	63
R(10-24)	1.798	A(10-24-19)	111.3
R(11-23)	1.647	A(11-23-17)	144.1
R(12-14)	1.632	A(11-23-19)	63.1
R(12-18)	1.625	A(14-12-18)	135
R(13-15)	1.625	A(12-14-16)	63
R(13-19)	1.632	A(12-14-25)	135
R(14-16)	1.798	A(12-18-22)	63.3
R(14-25)	1.625	A(12-18-24)	135
R(15-17)	1.808	A(15-13-19)	135
R(15-25)	1.632	A(13-15-17)	63.3
R(16-20)	1.647	A(13-15-25)	135
R(16-22)	1.647	A(13-19-23)	63
R(17-21)	1.647	A(13-19-24)	135
R(17-23)	1.647	A(16-14-25)	111.3
R(18-22)	1.808	A(14-16-20)	63.1
R(18-24)	1.632	A(14-16-22)	114.3

R(19-23)	1.798	A(14-25-15)	135
R(19-24)	1.625	A(14-25-21)	111.3
R(20-21)	1.647	A(17-15-25)	114.5
R(21-25)	1.798	A(15-17-21)	62.5
A(3-1-5)	135	A(15-17-23)	109.8
A(1-3-8)	135	A(15-25-21)	63
A(1-3-16)	63.1	A(20-16-22)	144.1
A(1-3-26)	68.4	A(16-20-21)	125.9
A(1-5-7)	135	A(16-22-18)	109.8
A(1-5-22)	63.5	A(21-17-23)	125.9
A(1-5-26)	68.5	A(17-21-20)	144.1
A(4-2-6)	135	A(17-21-25)	114.3
A(2-4-8)	135	A(17-23-19)	114.3
A(2-4-17)	63.5	A(22-18-24)	114.5
A(2-4-26)	68.5	A(18-24-19)	135
A(2-6-7)	135	A(23-19-24)	111.3
A(2-6-23)	63.1	A(20-21-25)	63.1
A(2-6-26)	68.4	A(4-26-6)	85.4
A(8-3-16)	111.3	A(7-5-22)	114.4
A(8-3-26)	68.5	A(7-5-26)	68.4
A(3-8-4)	135	A(5-7-6)	135
A(3-8-21)	111.3	A(5-7-10)	63.1
A(16-3-26)	68.8	A(22-5-26)	73.2
A(3-16-14)	125.6	A(5-22-10)	62.5
A(3-16-20)	63.4	A(5-22-16)	109.5
A(3-16-22)	114.4	A(5-22-18)	124.1
A(3-26-4)	85.4	A(5-26-6)	85.4
A(3-26-5)	85.4	A(7-6-23)	111.3
A(3-26-6)	147.3	A(7-6-26)	68.5
A(8-4-17)	114.4	A(6-7-10)	111.3
A(8-4-26)	68.4	A(23-6-26)	68.8
A(4-8-21)	63.1	A(6-23-11)	63.4
A(17-4-26)	73.2	A(6-23-17)	114.4
A(4-17-15)	124.1	A(6-23-19)	125.6
A(4-17-21)	62.5	A(7-10-11)	63.4
A(4-17-23)	109.5	A(7-10-22)	114.4
A(4-26-5)	147.3	A(7-10-24)	125.6
A(8-21-25)	125.6	A(8-21-17)	114.4
A(14-9-15)	88	A(8-21-20)	63.4

Co₂B₂₄⁻

R(1-8)	2.207	R(5-12)	1.62
R(1-12)	2.207	R(5-16)	1.609
R(1-15)	2.207	R(6-9)	1.65
R(1-16)	2.207	R(6-12)	1.797
R(1-26)	2.681	R(6-17)	1.65
R(2-8)	1.62	R(6-23)	1.802
R(2-13)	1.782	R(7-8)	1.609
R(2-15)	1.609	R(7-14)	1.782
R(3-9)	1.65	R(7-16)	1.62
R(3-14)	1.65	R(8-11)	1.797
R(3-16)	1.797	R(9-19)	1.785
R(3-25)	1.802	R(10-12)	1.609
R(4-13)	1.65	R(10-15)	1.62
R(4-15)	1.797	R(10-17)	1.782
R(4-17)	1.65	R(11-13)	1.65
R(4-24)	1.802	R(11-14)	1.65
R(5-9)	1.782	R(11-21)	1.802
R(19-25)	1.619	R(13-18)	1.785
R(20-21)	1.619	R(14-20)	1.785
R(20-25)	1.624	R(17-22)	1.785
R(21-26)	2.125	R(18-21)	1.624
R(22-23)	1.619	R(18-24)	1.619
R(22-24)	1.624	R(19-23)	1.624
R(23-26)	2.125	R(24-26)	2.125
R(25-26)	2.125	A(1-26-25)	85.7
A(8-1-12)	145.9	A(8-2-13)	63
A(8-1-15)	85.1	A(8-2-15)	135
A(8-1-16)	85.1	A(2-8-7)	135
A(8-1-26)	107	A(2-8-11)	115.2
A(1-8-2)	68.5	A(13-2-15)	111.5
A(1-8-7)	68.6	A(2-13-4)	63
A(1-8-11)	73.5	A(2-13-11)	114.5
A(12-1-15)	85.1	A(2-13-18)	125.4
A(12-1-16)	85.1	A(2-15-4)	63.4
A(12-1-26)	107	A(2-15-10)	135
A(1-12-5)	68.5	A(9-3-14)	124.2
A(1-12-6)	73.5	A(9-3-16)	108.9
A(1-12-10)	68.6	A(9-3-25)	109
A(15-1-16)	145.9	A(3-9-5)	63
A(15-1-26)	107	A(3-9-6)	145.8
A(1-15-2)	68.6	A(3-9-19)	63.2
A(1-15-4)	73.5	A(14-3-16)	62.1

A(1-15-10)	68.5	A(14-3-25)	62.1
A(16-1-26)	107	A(3-14-7)	114.5
A(1-16-3)	73.5	A(3-14-11)	145.8
A(1-16-5)	68.6	A(3-14-20)	114.7
A(1-16-7)	68.5	A(16-3-25)	123.4
A(1-26-21)	85.7	A(3-16-5)	63.4
A(1-26-23)	85.7	A(3-16-7)	115.2
A(1-26-24)	85.7	A(3-25-19)	63.3
A(3-25-20)	115.1	A(9-6-12)	62.1
A(3-25-26)	91.9	A(9-6-17)	124.2
A(13-4-15)	108.9	A(9-6-23)	62.1
A(13-4-17)	124.2	A(6-9-19)	114.7
A(13-4-24)	109	A(12-6-17)	108.9
A(4-13-11)	145.8	A(12-6-23)	123.4
A(4-13-18)	63.2	A(6-12-10)	63.4
A(15-4-17)	62.1	A(17-6-23)	109
A(15-4-24)	123.4	A(6-17-10)	63
A(4-15-10)	115.2	A(6-17-22)	63.2
A(17-4-24)	62.1	A(6-23-19)	115.1
A(4-17-6)	145.8	A(6-23-22)	63.3
A(4-17-10)	114.5	A(6-23-26)	91.9
A(4-17-22)	114.7	A(8-7-14)	111.5
A(4-24-18)	63.3	A(8-7-16)	135
A(4-24-22)	115.1	A(7-8-11)	63.4
A(4-24-26)	91.9	A(14-7-16)	63
A(9-5-12)	63	A(7-14-11)	63
A(9-5-16)	111.5	A(7-14-20)	125.4
A(5-9-6)	114.5	A(8-11-13)	62.1
A(5-9-19)	125.4	A(8-11-14)	108.9
A(12-5-16)	135	A(8-11-21)	123.4
A(5-12-6)	115.2	A(9-19-23)	62.9
A(5-12-10)	135	A(9-19-25)	111.3
A(5-16-7)	135	A(12-10-15)	135
A(11-21-18)	115.1	A(12-10-17)	111.5
A(11-21-20)	63.3	A(15-10-17)	63
A(11-21-26)	91.9	A(10-17-22)	125.4
A(13-18-21)	62.9	A(13-11-14)	124.2
A(13-18-24)	111.3	A(13-11-21)	62.1
A(14-20-21)	111.3	A(11-13-18)	114.7
A(14-20-25)	62.9	A(14-11-21)	109
A(17-22-23)	111.3	A(11-14-20)	63.2
A(17-22-24)	62.9	W4(B1)	230.3
A(21-18-24)	135	W5(A1)	234
A(18-21-20)	135	W6(B2)	261.4

A(18-21-26)	67.5	W7(E)	285.2
A(18-24-22)	135	W8(E)	285.2
A(18-24-26)	67.6	W9(B1)	289.1
A(23-19-25)	135	W10(B2)	312.7
A(19-23-22)	135	W11(A2)	321.9
A(19-23-26)	67.5	W12(A1)	345.3
A(19-25-20)	135	W13(E)	347.5
A(19-25-26)	67.6	W14(E)	347.5
A(21-20-25)	135	W15(A2)	366.4
A(20-21-26)	67.6	W16(E)	381.4
A(20-25-26)	67.5	W17(E)	381.4
A(21-26-23)	171.5	W18(B2)	408.1
A(21-26-24)	89.7	W19(E)	418.2
A(21-26-25)	89.7	W20(E)	418.2
A(23-22-24)	135	W21(B1)	423.8
A(22-23-26)	67.6	W22(A2)	433
A(22-24-26)	67.5	W23(B1)	440.4
A(23-26-24)	89.7	W24(B2)	449
A(23-26-25)	89.7	W25(E)	468.2
A(24-26-25)	171.5	W26(E)	468.2
W1(A1)	180.5	W27(E)	476.2
W2(E)	187.8	W28(E)	476.2
W3(E)	187.8	W29(A1)	479.8
W41(A1)	616.1	W30(E)	502.4
W42(B1)	656.7	W31(E)	502.4
W43(E)	659.8	W32(E)	518.2
W44(E)	659.8	W33(E)	518.2
W45(A1)	666	W34(B1)	525.8
W46(B2)	667.3	W35(B2)	526.3
W47(A1)	687.7	W36(E)	528
W48(A2)	698.7	W37(E)	528
W49(E)	731.2	W38(A2)	534.2
W50(E)	731.2	W39(A2)	564.8
W51(E)	749.3	W40(A1)	595.7
W52(E)	749.3	W62(E)	1025
W53(A1)	805.2	W63(B2)	1028.5
W54(E)	851.6	W64(B1)	1042.4
W55(E)	851.6	W65(B1)	1060.6
W56(E)	866.1	W66(A2)	1115.1
W57(E)	866.1	W67(E)	1158.3
W58(B2)	902	W68(E)	1158.3
W59(B1)	997.5	W69(A1)	1191
W60(B2)	1009.8	W70(E)	1205.1
W61(E)	1025	W71(E)	1205.1

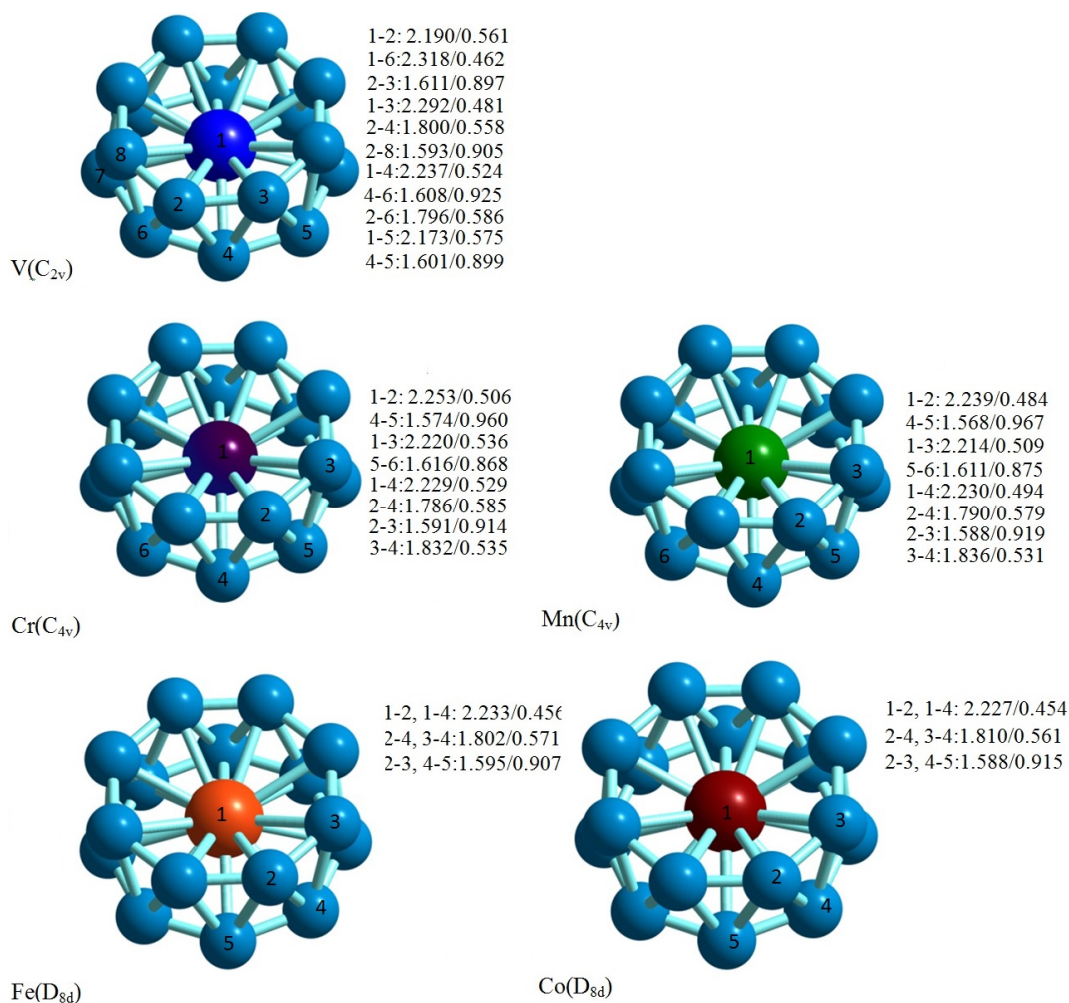
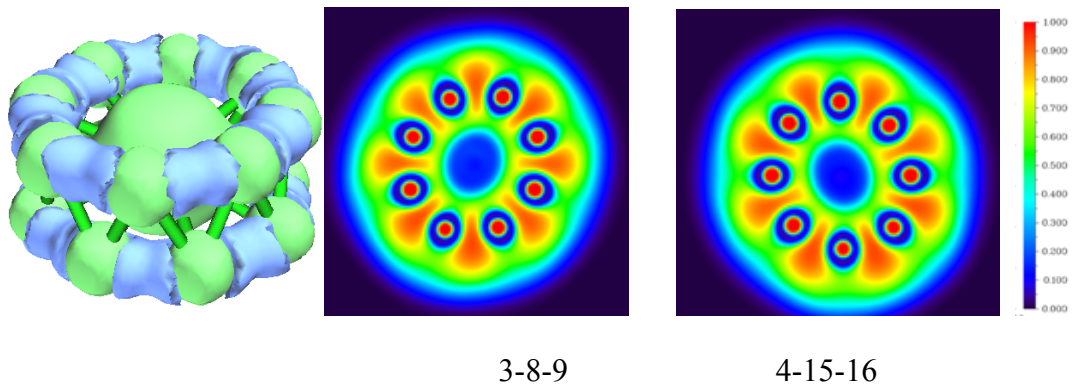
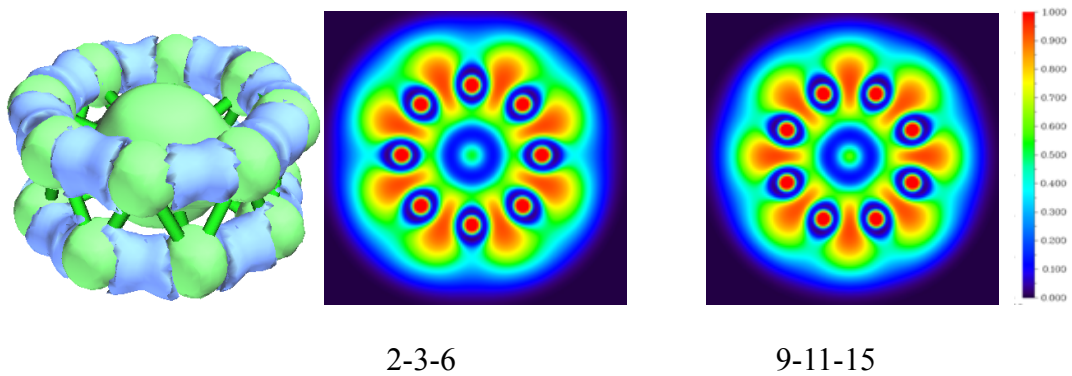


Fig. S1 Structures and selected bond length in Å of global minima of MB₁₆⁻ clusters. Wiberg bond indices are given after the backslash.

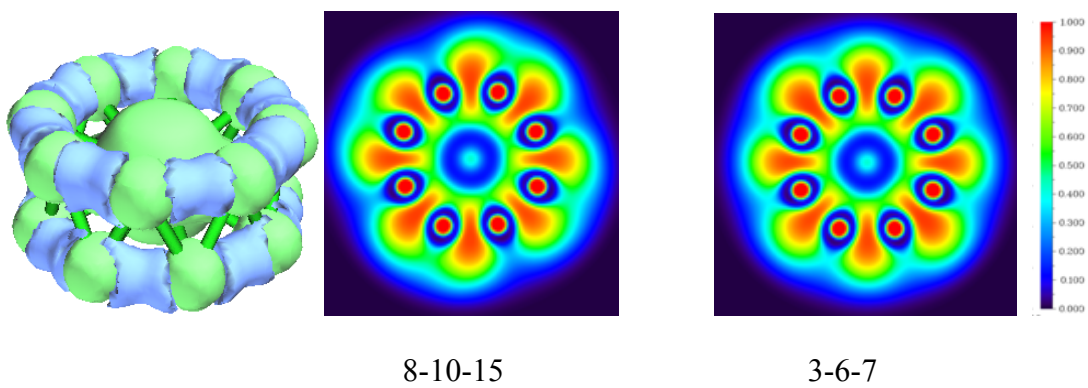
$\text{VB}_{16}^{-} (\text{C}_{2v})$



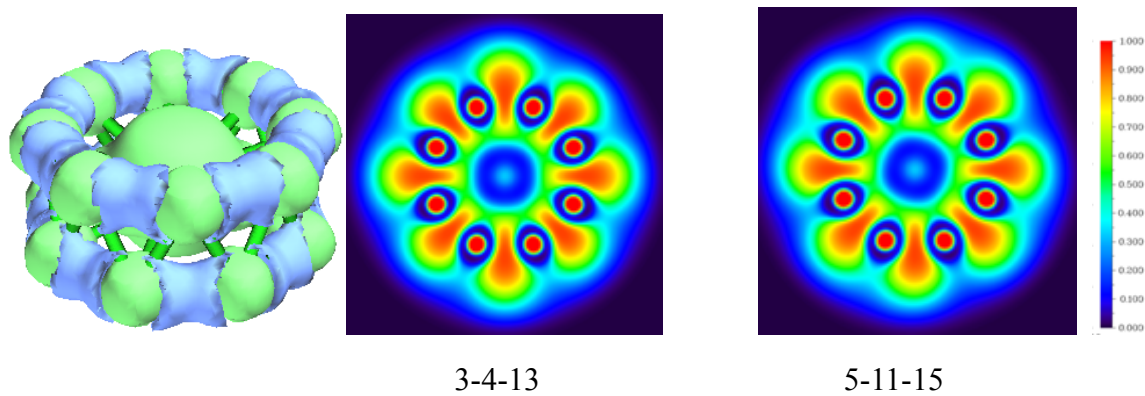
$\text{CrB}_{16}^{-} (\text{C}_{4v})$



$\text{MnB}_{16}^{-} (\text{C}_{4v})$



$\text{FeB}_{16}^- (\text{D}_{8d})$



$\text{CoB}_{16}^- (\text{D}_{8d})$

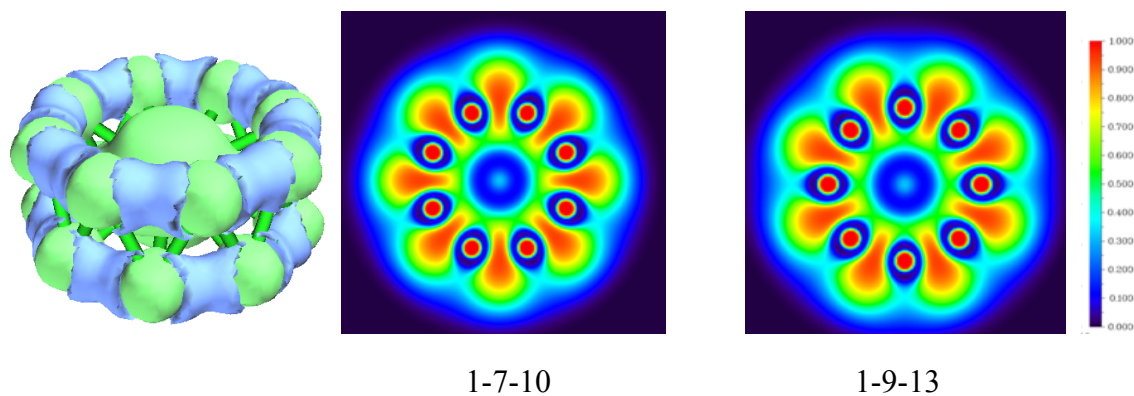


Fig. S2 Isosurface of electron localization function (ELF) with the value of 0.70 and the contour plots of ELF within different plane of highly symmetric structures of $\text{VB}_{16}^- (\text{C}_{2v})$, $\text{CrB}_{16}^- (\text{C}_{4v})$, $\text{MnB}_{16}^- (\text{C}_{4v})$, $\text{FeB}_{16}^- (\text{D}_{8d})$, and $\text{CoB}_{16}^- (\text{D}_{8d})$, respectively.

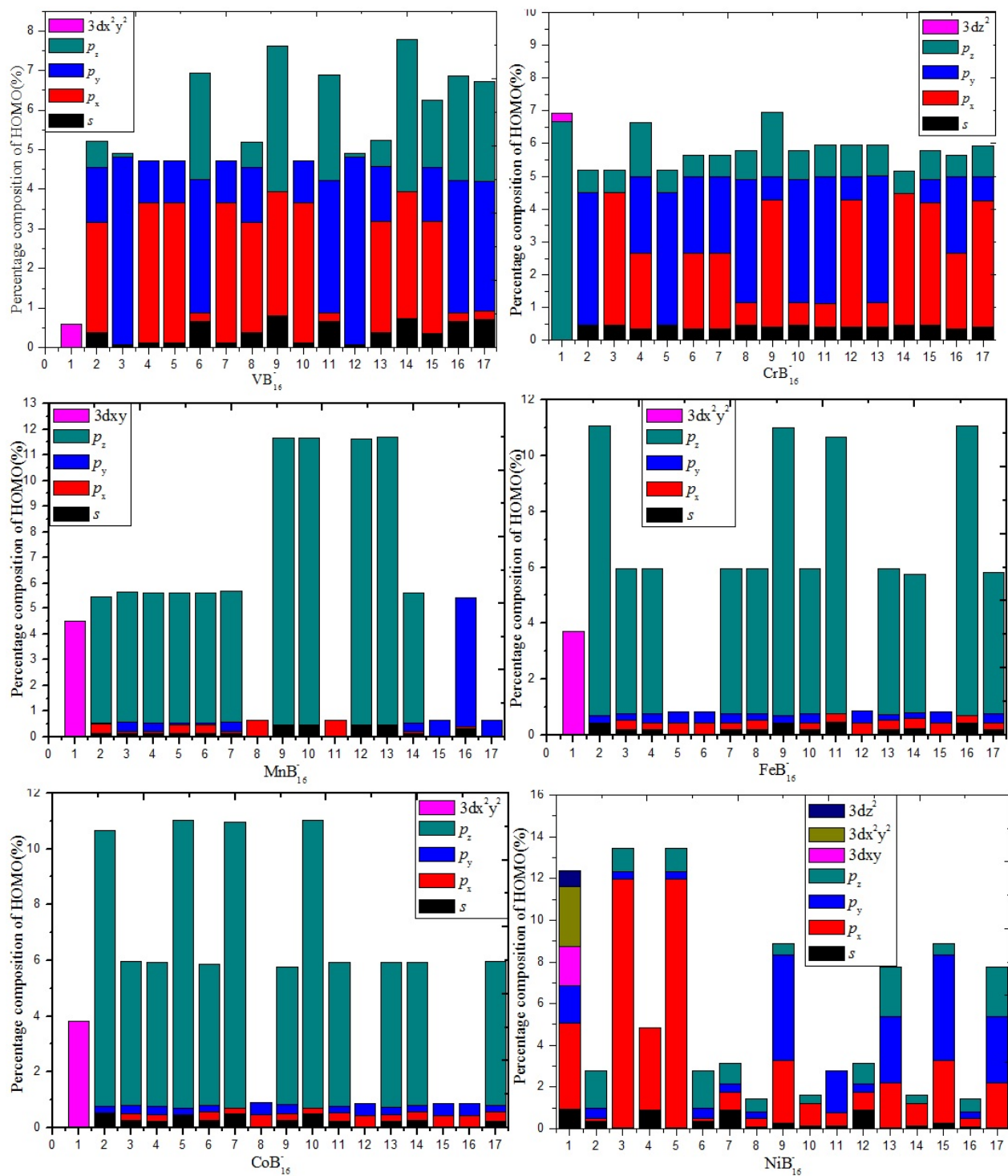


Figure S3. Contributions (%) of TM atoms and boron atoms to the highest occupied molecular orbital (HOMO) of MB_{16}^- ($M=V, Cr, Mn, Fe, Co, Ni$) clusters.

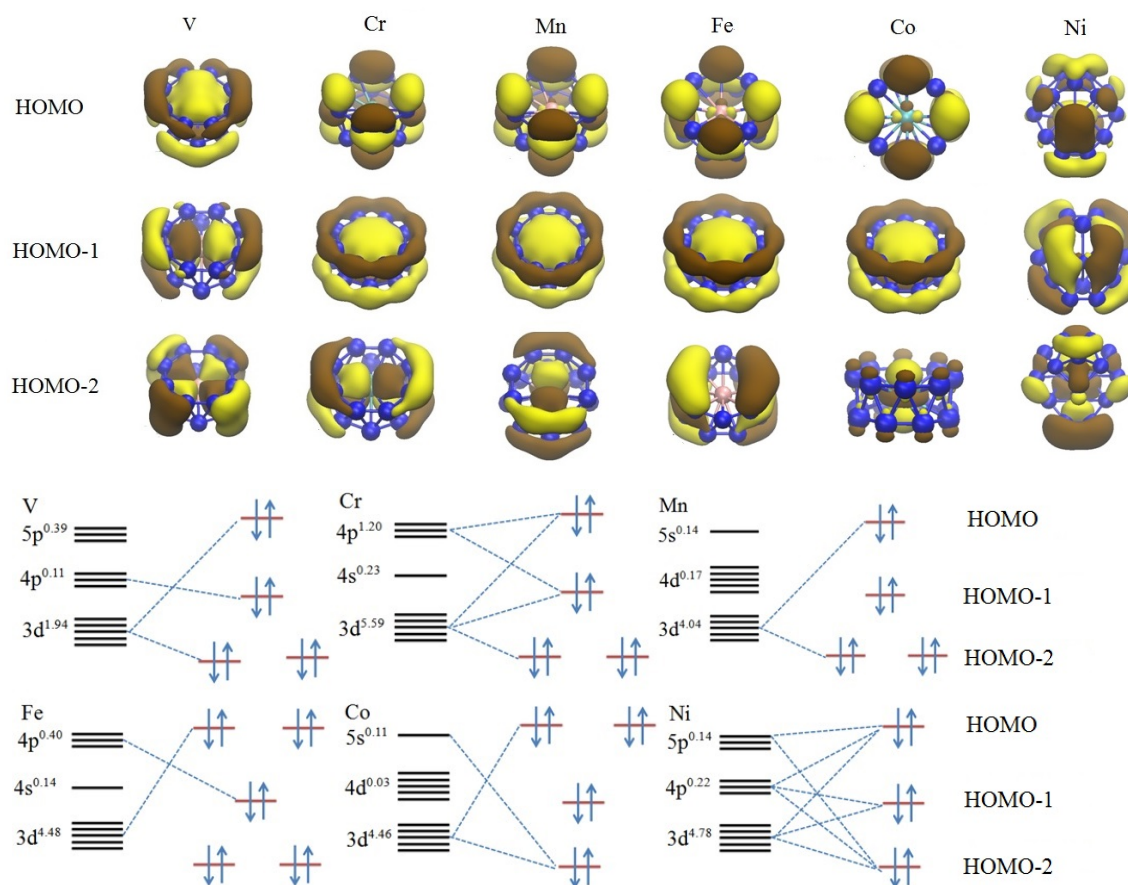


Figure S4. Chemical bonding in MB_{16}^- ($M=V, Cr, Mn, Fe, Co, Ni$) clusters. (a) Valence MOs (b) Correlation diagram for the valence MOs.

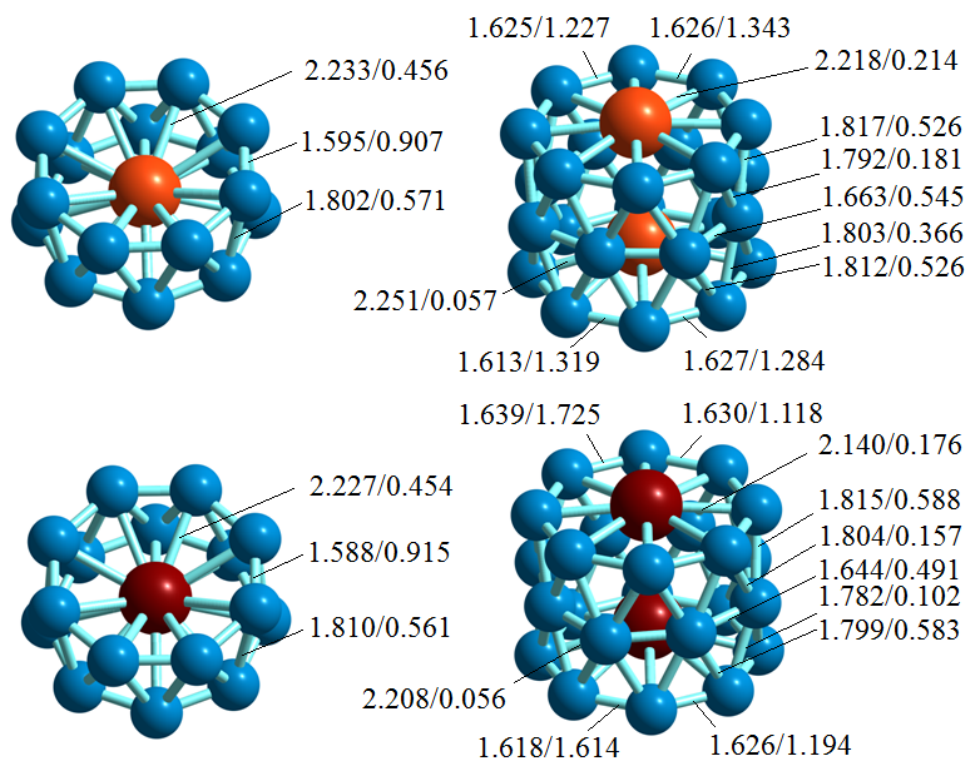


Fig. S5 Structures and selected bond length in Å of global minima of $\text{Fe}_2\text{B}_{24}^-$ and $\text{Co}_2\text{B}_{24}^-$ clusters.

Wiberg bond indices are given after the backslash.