Electronic Supplementary Material (ESI) for Nanoscale.

Stabilization of Fullerene-like Boron Cages by Transition Metal Encapsulation

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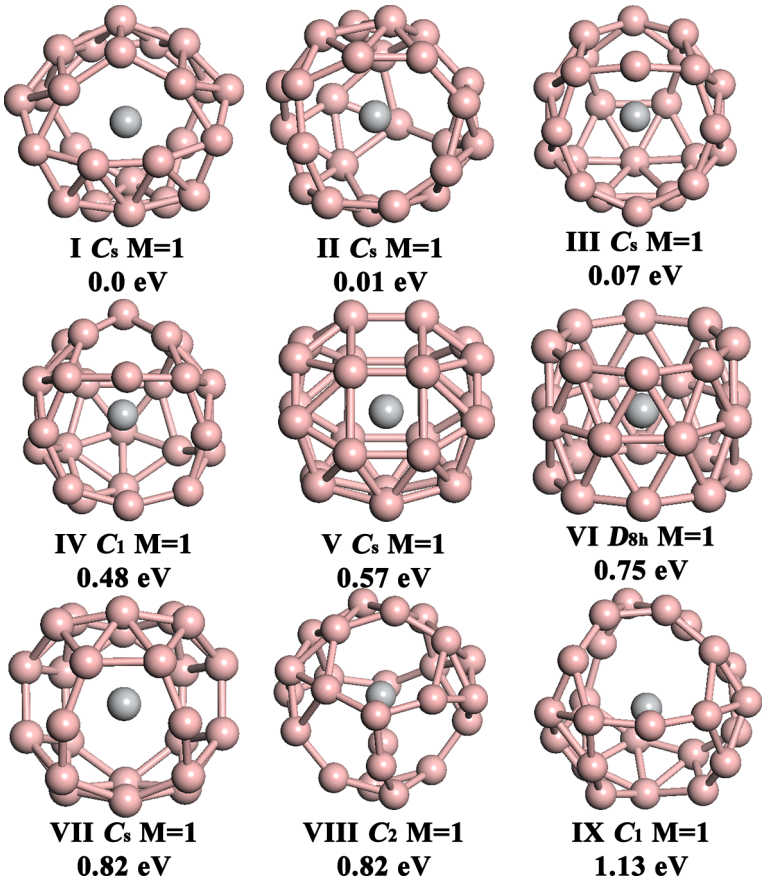

Fig. S1 Structures of low-lying isomers of TiB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Ti/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

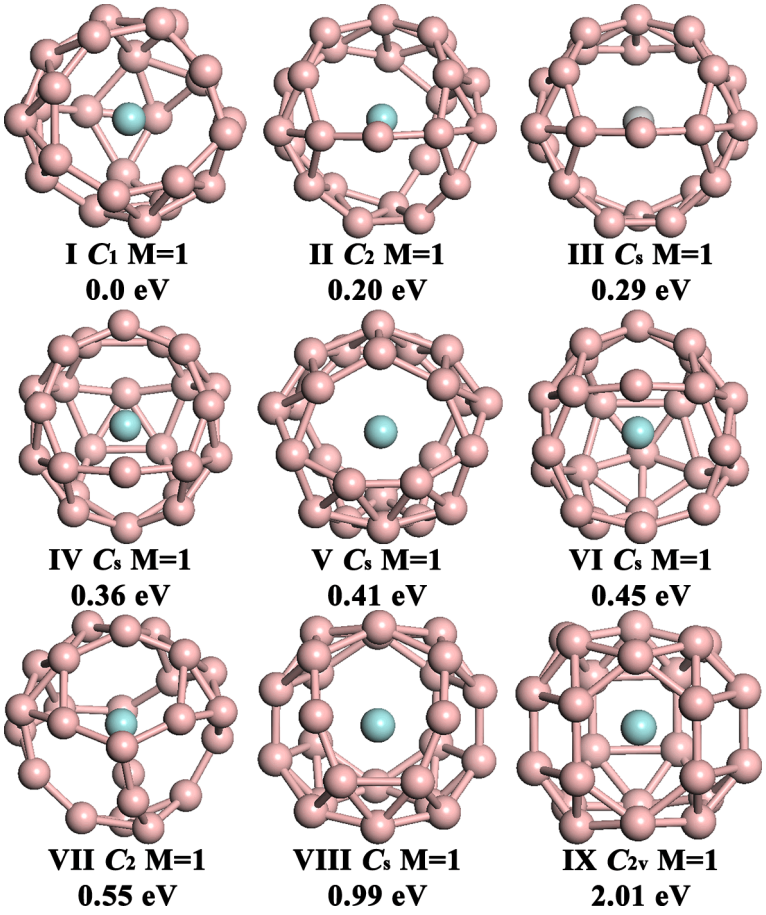

Fig. S2 Structures of low-lying isomers of ZrB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Zr/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

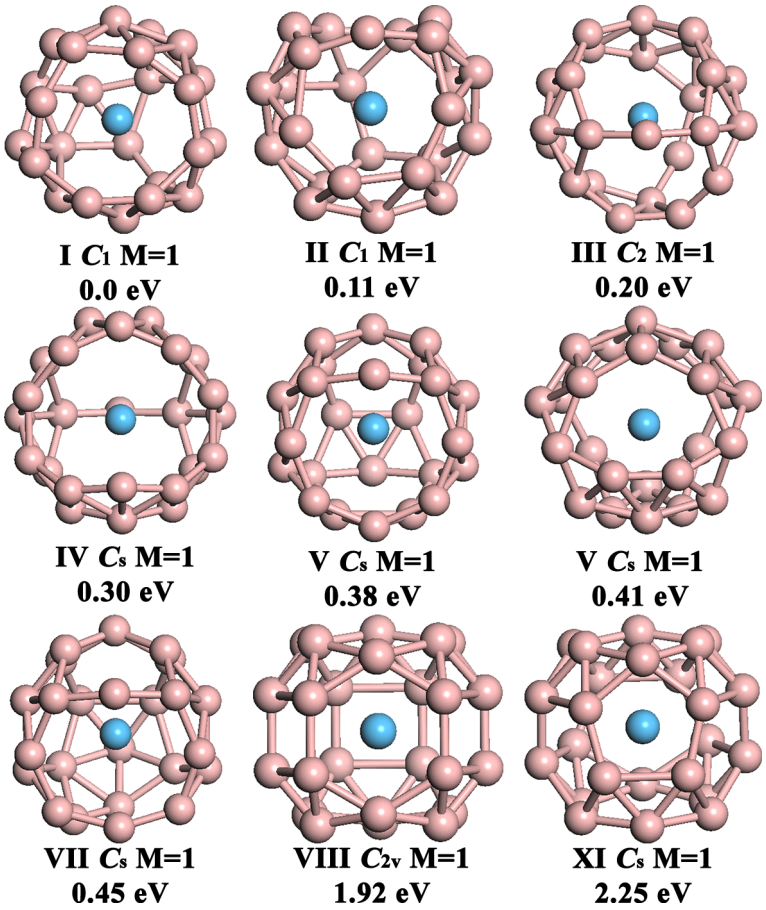

Fig. S3 Structures of low-lying isomers of HfB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Hf/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

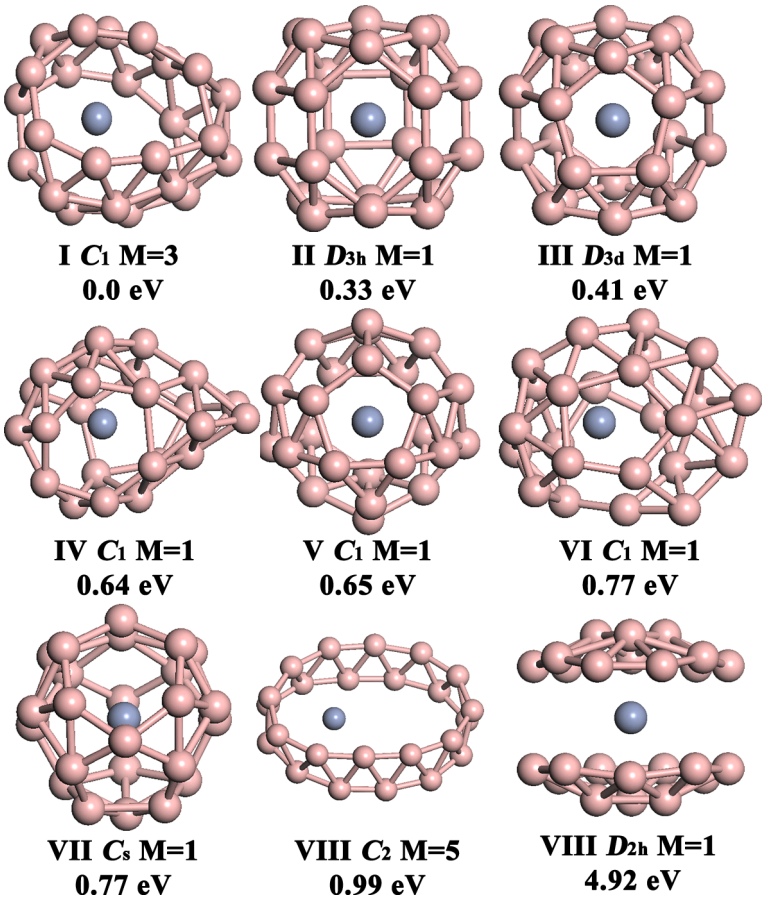

Fig. S4 Structures of low-lying isomers of CrB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Cr/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

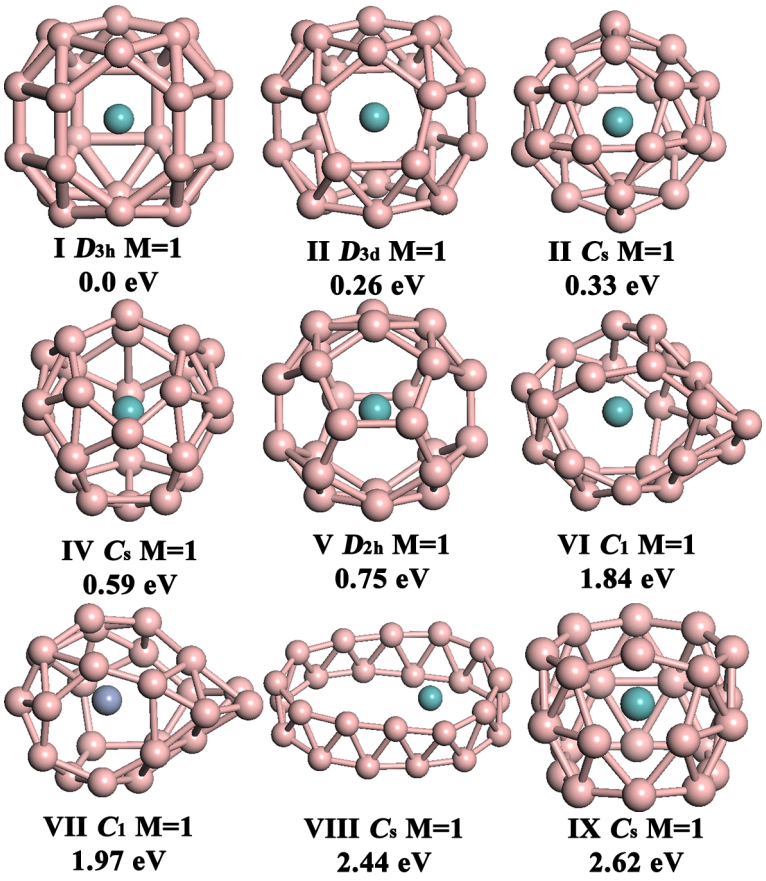

Fig. S5 Structures of low-lying isomers of MoB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Mo/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

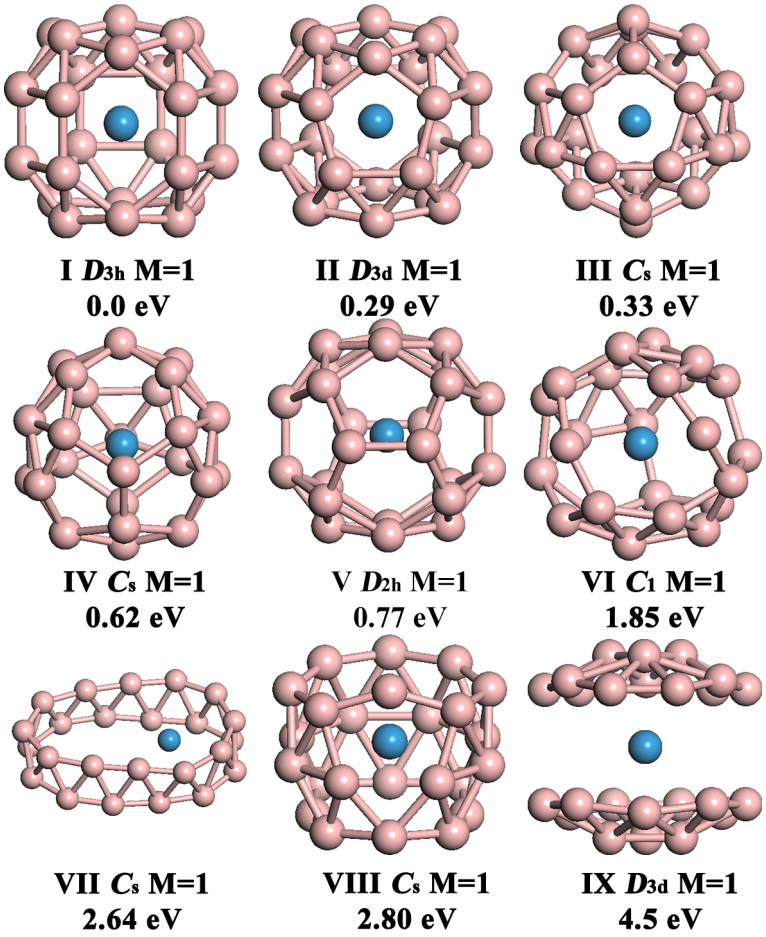

Fig. S6 Structures of low-lying isomers of WB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/W/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

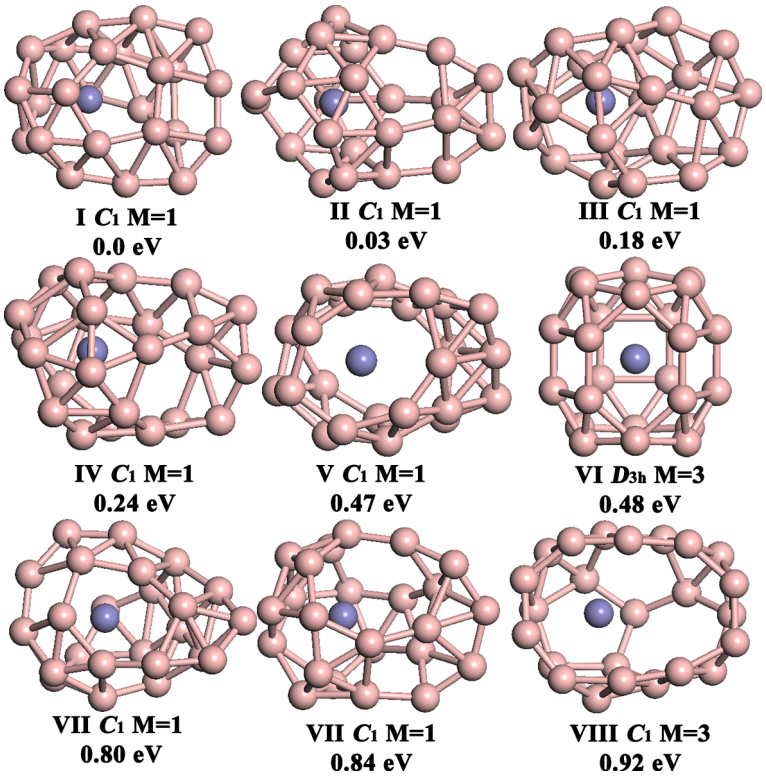

Fig. S7 Structures of low-lying isomers of FeB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Fe/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

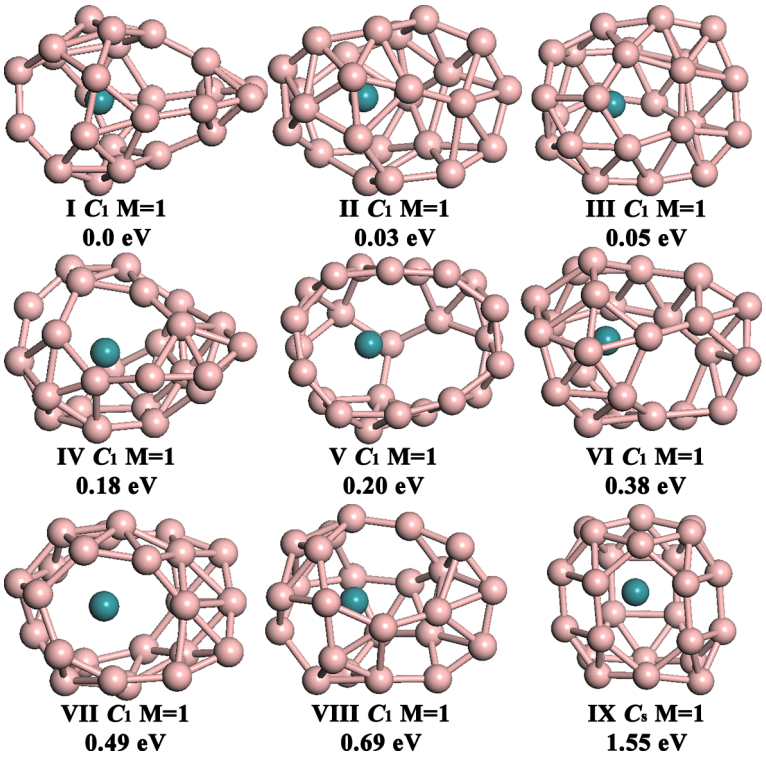

Fig. S8 Structures of low-lying isomers of RuB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Ru/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

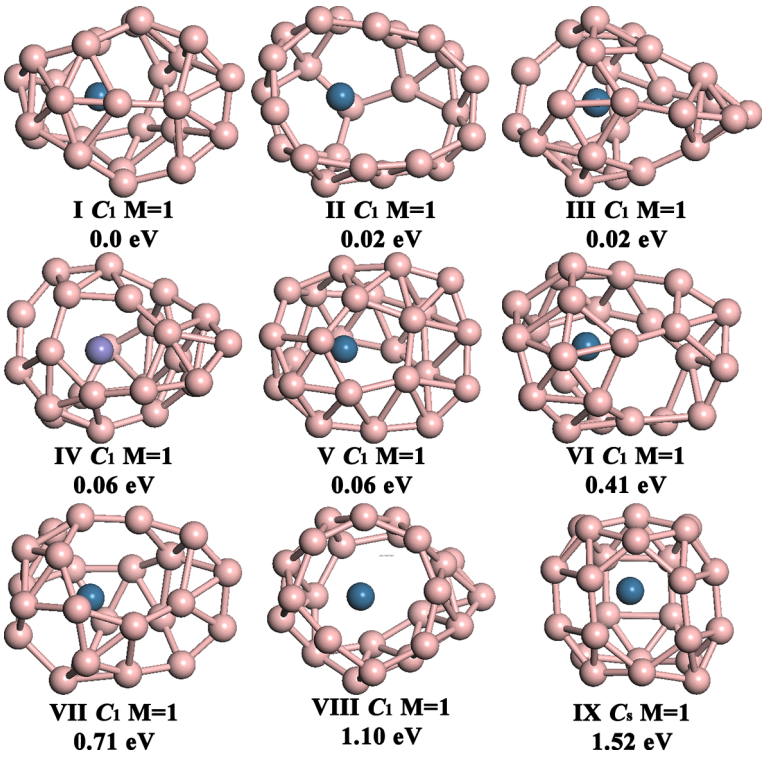

Fig. S9 Structures of low-lying isomers of OsB_{24}. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Os/Stuttgart/B/6-311G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

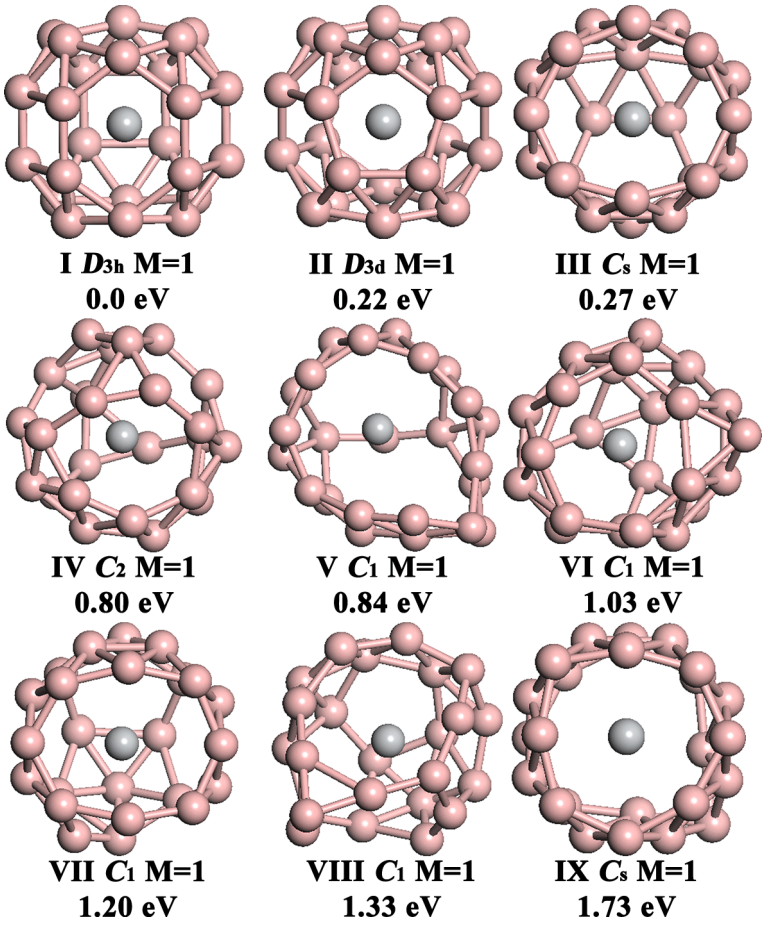

Fig. S10 Structures of TiB_{24}^{2-} derived by re-optimizations of low-lying isomers of TiB_{24} in Fig. S1. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Ti/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

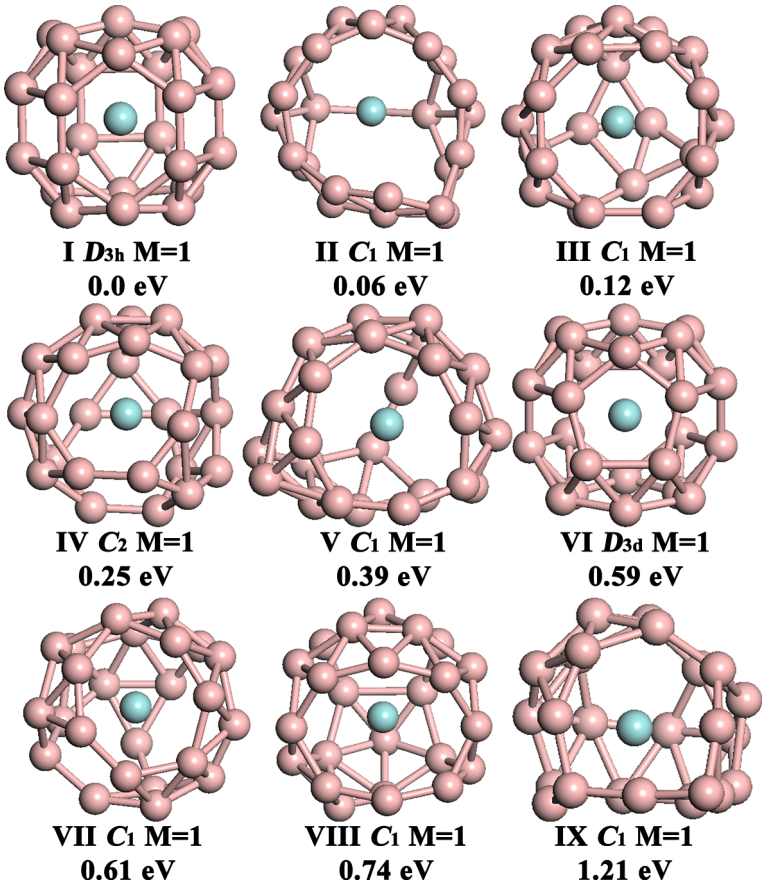

Fig. S11 Structures of ZrB_{24}^{2-} derived by re-optimizations of low-lying isomers of ZrB_{24} in Fig. S2. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Zr/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

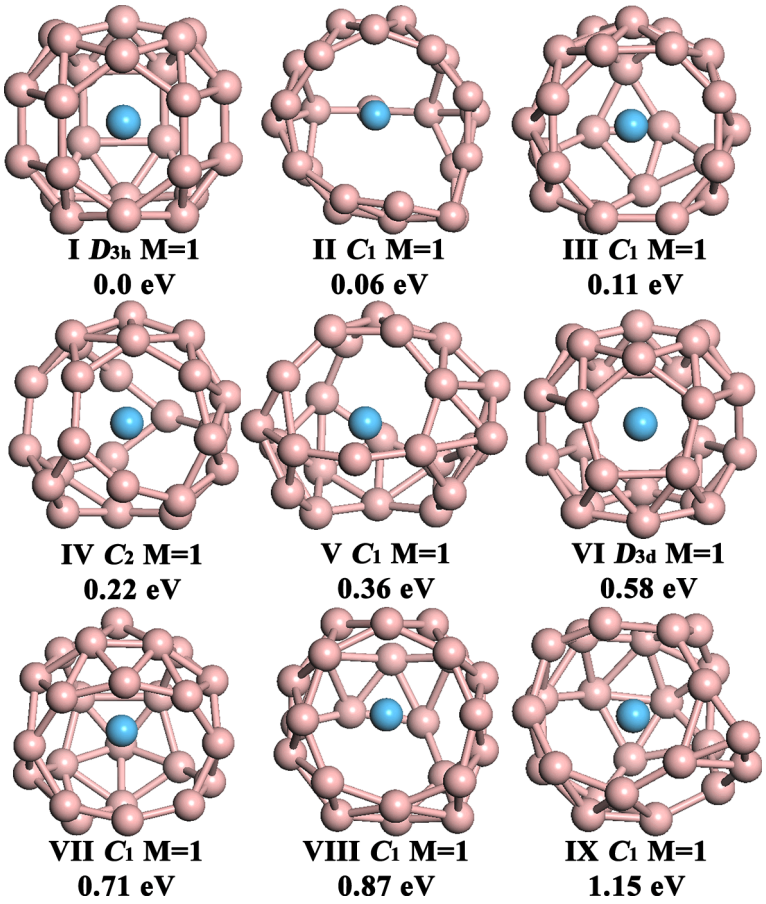

Fig. S12 Structures of HfB_{24}^{2-} derived by re-optimizations of low-lying isomers of HfB_{24} in Fig. S3. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Hf/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

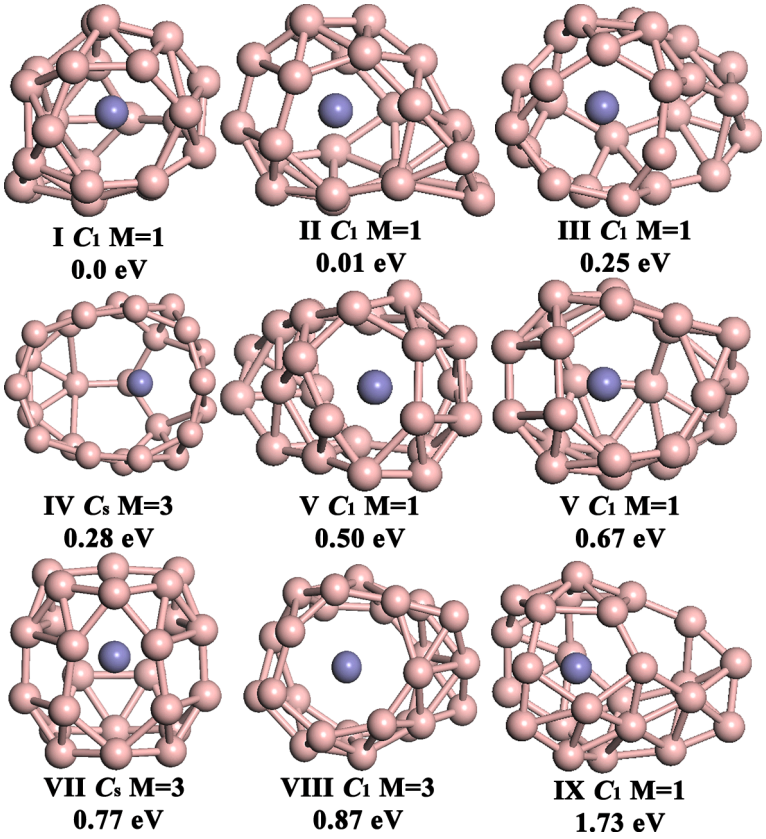

Fig. S13 Structures of FeB_{24}^{2+} derived by re-optimizations of low-lying isomers of FeB_{24} in Fig. S7. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Fe/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

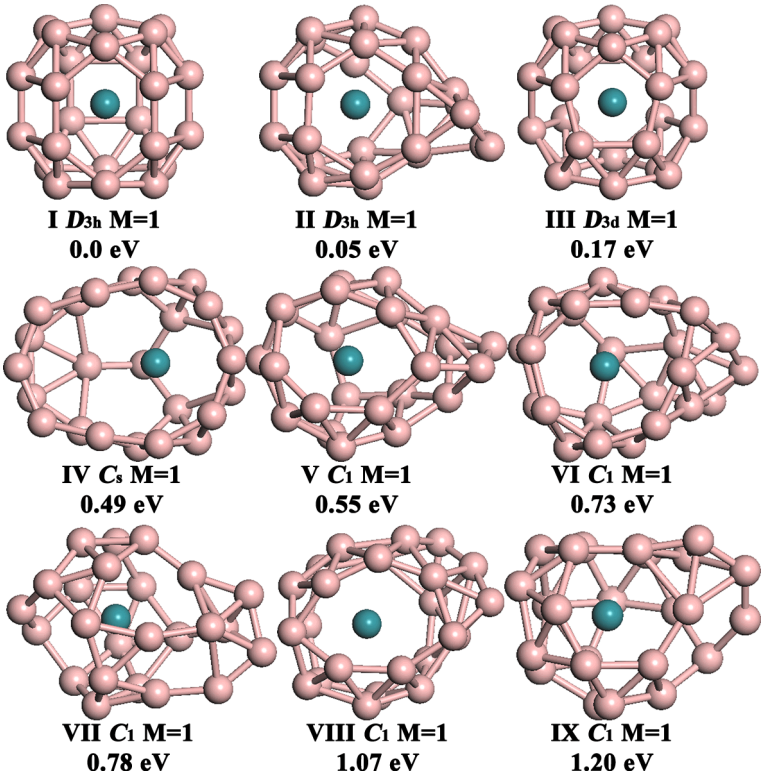

Fig. S14 Structures of RuB_{24}^{2+} derived by re-optimizations of low-lying isomers of RuB_{24} in Fig. S8. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Ru/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

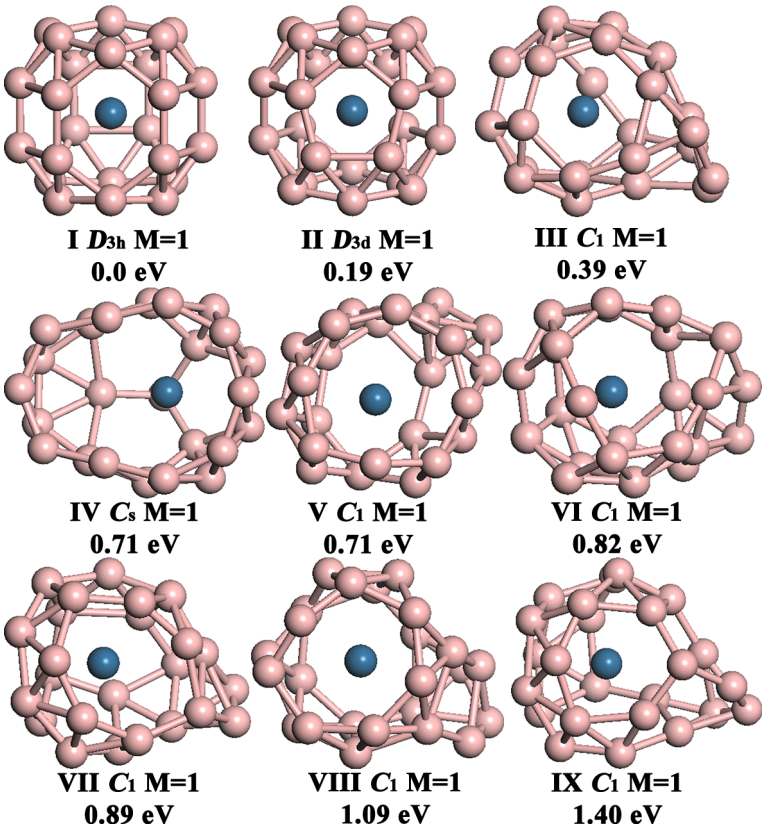

Fig. S15 Structures of OsB_{24}^{2+} derived by re-optimizations of low-lying isomers of OsB_{24} in Fig. S9. Bottom labels are point-group symmetries, spin multiplicities and relative energies to the ground state at PBE0/Os/Stuttgart/B/6-311+G* level of theory, zero-point energy corrections were included for all isomers at the same level of theory.

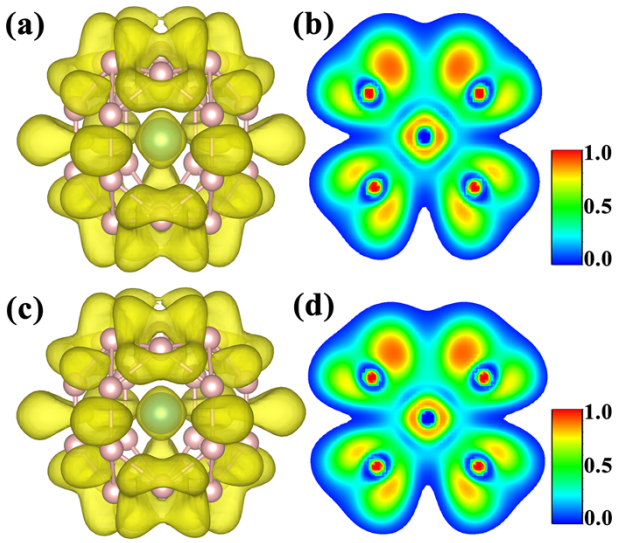

Fig. S16 Isosurface of electron localization function (ELF) with the value of 0.75 and the contour plots of ELF within one plane through the principal axis of the endohedral D_{3h} cage for MoB_{24} (a, b) and WB_{24} (c, d), respectively.

Table SI. Cartesian coordinates of the lowest-energy structure of TiB_{24}.

Ti	9.871201096	10.004686800	9.916963827
B	8.017614213	11.403722002	9.025625523
B	7.795576088	9.462194308	11.509474517
B	10.354033482	8.079879413	8.632580850
B	11.213158720	8.145690420	10.292752912
B	11.729257992	10.798946224	11.510169189
B	9.437407681	9.574588950	7.640288699
B	11.717429188	11.418030920	10.028718162
B	8.525399839	8.063867972	11.188371370
B	11.172135108	9.240908082	11.704358052
B	10.231796936	10.761950238	12.088394583
B	8.632627052	10.897855570	11.855256608
B	10.121349103	8.012614448	11.494620180
B	10.697644088	10.743797308	7.486055517
B	9.339127152	11.372354615	8.015052998
B	8.010367022	9.740375959	8.490562901
B	11.069782000	9.187510771	7.660847022
B	11.928684732	8.810764859	8.988935093
B	7.812419447	8.856966277	9.893167865
B	9.447127056	7.679373981	9.889913396
B	12.143801720	9.670012721	10.357242166
B	9.423959653	12.399931820	9.353976760
B	8.531429225	12.005775077	10.591378461
B	10.898420971	11.898469024	8.713966223
B	7.601168436	10.604842240	10.424554125

Table SII. Cartesian coordinates of the lowest-energy structure of ZrB_{24}.

Zr	9.279053000	9.892326000	9.672086000
B	7.542308000	8.284460000	8.752212000
B	11.605693000	9.195025000	8.686871000
B	9.149004000	12.150518000	8.387590000
B	7.875521000	11.667722000	10.845465000
B	9.512331000	7.720524000	10.770982000
B	11.113449000	10.345072000	11.238253000
B	7.749008000	8.959726000	11.403035000
B	10.615873000	8.708709000	11.487259000
B	9.517796000	11.476199000	11.493894000
B	7.995607000	11.067548000	7.841545000
B	10.439872000	8.068407000	8.448260000
B	10.640030000	11.843145000	9.015528000
B	9.817952000	10.018498000	12.178996000
B	8.993162000	8.421902000	7.691959000
B	7.743319000	11.922168000	9.299716000
B	9.067700000	7.475064000	9.169674000
B	11.655350000	10.686962000	9.591120000
B	7.900255000	7.807796000	10.346104000
B	11.713120000	9.158179000	10.270046000
B	9.349396000	12.325368000	10.057558000
B	7.616458000	9.464664000	7.724025000
B	10.404879000	9.460757000	7.488133000
B	9.831325000	11.014606000	7.532063000
B	8.193442000	10.419950000	11.912116000

Table SIII. Cartesian coordinates of the lowest-energy structure of HfB_{24}.

Hf	9.273876000	9.891929000	9.671259000
B	7.542868000	8.283480000	8.750481000
B	11.604708000	9.195094000	8.687288000
B	9.150050000	12.149146000	8.387775000
B	7.876820000	11.669122000	10.844311000
B	9.514536000	7.719419000	10.769634000
B	11.112629000	10.344705000	11.236768000
B	7.746821000	8.959733000	11.405556000
B	10.615672000	8.709242000	11.486454000
B	9.518679000	11.477142000	11.493889000
B	7.994632000	11.067448000	7.842894000
B	10.439698000	8.068067000	8.448670000
B	10.640189000	11.842812000	9.016979000
B	9.818993000	10.019396000	12.179226000
B	8.992867000	8.419879000	7.692187000
B	7.742654000	11.923025000	9.299647000
B	9.068575000	7.473802000	9.169999000
B	11.655485000	10.686730000	9.590635000
B	7.901568000	7.810892000	10.346624000
B	11.715020000	9.159175000	10.269935000
B	9.349781000	12.326656000	10.058283000
B	7.616815000	9.464562000	7.725131000
B	10.403560000	9.460333000	7.488718000
B	9.831568000	11.014101000	7.532049000
B	8.193898000	10.419336000	11.910043000

Table SIV. Cartesian coordinates of the lowest-energy structure of CrB_{24}.

Cr	-0.436443000	0.133062000	-0.243270000
B	1.474247000	-0.925374000	1.409400000
B	-0.006190000	-1.536620000	1.527547000
B	-1.437179000	-0.844647000	1.409803000
B	-2.581102000	0.123185000	0.805035000
B	-1.178079000	1.145692000	1.440007000
B	0.463870000	1.384921000	1.601503000
B	1.920216000	0.617189000	2.024052000
B	2.942522000	-0.078869000	1.099267000
B	0.894077000	-1.891849000	0.158244000
B	-0.826082000	-1.965833000	0.042263000
B	-2.251243000	-1.155680000	-0.170500000
B	-2.355772000	1.611754000	0.266205000
B	-1.070478000	2.358781000	-0.157267000
B	0.578116000	2.137597000	0.011240000
B	1.695680000	0.949847000	0.296565000
B	2.675250000	-1.232049000	-0.028858000
B	1.918148000	-1.899417000	-1.229078000
B	0.303701000	-1.645633000	-1.463674000
B	-1.316755000	-1.524017000	-1.575545000
B	-2.078667000	-0.130447000	-1.653115000
B	-1.819346000	1.451463000	-1.414424000
B	-0.220371000	1.923138000	-1.558167000
B	1.231860000	1.294287000	-1.322370000
B	1.480023000	-0.300478000	-1.274866000

Table SV. Cartesian coordinates of the lowest-energy structure of MoB_{24}.

Mo	0.000002000	-0.000198000	0.000000000
B	1.284567000	-0.741648000	-2.039289000
B	1.515776000	0.875139000	-1.847749000
B	0.000000000	1.483296000	-2.039298000
B	-1.515774000	0.875138000	-1.847751000
B	-1.284568000	-0.741648000	-2.039290000
B	0.000000000	-1.750171000	-1.847428000
B	1.284569000	-0.741649000	2.039289000
B	1.515775000	0.875139000	1.847749000
B	0.000000000	1.483296000	2.039298000
B	-1.515775000	0.875138000	1.847751000
B	-1.284569000	-0.741649000	2.039290000
B	0.000000000	-1.750170000	1.847429000
B	1.346627000	-1.844010000	0.818204000
B	2.270194000	-0.244013000	0.818217000
B	0.923773000	2.088021000	0.818221000
B	-0.923776000	2.088019000	0.818221000
B	-2.270193000	-0.244013000	0.818217000
B	-1.346628000	-1.844010000	0.818205000
B	2.270193000	-0.244015000	-0.818218000
B	0.923774000	2.088021000	-0.818221000
B	-0.923775000	2.088020000	-0.818220000
B	-2.270192000	-0.244013000	-0.818217000
B	-1.346629000	-1.844009000	-0.818205000
B	1.346628000	-1.844010000	-0.818205000

Table SVI. Cartesian coordinates of the lowest-energy structure of WB_{24}.

W	9.592424560	9.779479600	9.526255760
B	8.132035392	9.920824442	7.474716873
B	8.574249422	8.349222196	7.683771356
B	10.209243325	8.405971041	7.502759889
B	11.348349478	9.578429303	7.695034284
B	10.482655741	10.962387176	7.484260461
B	8.896918882	11.366193502	7.661939135
B	8.100928206	9.953661869	11.552736911
B	8.546086687	8.378951396	11.375786359
B	10.178136139	8.438808468	11.580779927
B	11.320186743	9.608158503	11.387049288
B	10.451548556	10.995224603	11.562280499
B	8.868756148	11.395922702	11.353954138
B	7.601345164	10.928877878	10.320688253
B	7.404527243	9.088623089	10.334005201
B	9.588788566	7.495698450	10.363493474
B	11.280899758	8.245474976	10.370363496
B	11.568403073	10.933641530	10.350910660
B	10.073109802	12.024119793	10.330723691
B	7.417018494	9.075437050	8.696455130
B	9.601279818	7.482512412	8.725943403
B	11.293391010	8.232288938	8.732813424
B	11.580894325	10.920455491	8.713360588
B	10.085601053	12.010933754	8.693173619
B	7.613836415	10.915691839	8.683138182

Table SVII. Cartesian coordinates of the lowest-energy structure of FeB_{24}.

Fe	10.768064000	9.908700000	10.410097000
B	7.503095000	8.928471000	9.043323000
B	8.984589000	9.781582000	8.561930000
B	10.309640000	7.569094000	9.182569000
B	11.322394000	7.583744000	7.789618000
B	9.959285000	9.987064000	12.451954000
B	12.433290000	11.209711000	9.738682000
B	10.709846000	8.497936000	12.109999000
B	12.847431000	9.590356000	9.719790000
B	11.656326000	9.814813000	12.324463000
B	12.669536000	10.411788000	11.188235000
B	10.436936000	11.415831000	11.920610000
B	11.562608000	11.888231000	10.881709000
B	9.000502000	10.760336000	11.205008000
B	10.894882000	11.706864000	9.289782000
B	9.171041000	9.004618000	11.385991000
B	11.682436000	10.347754000	8.548527000
B	8.464628000	8.097422000	8.116900000
B	9.839145000	7.553053000	7.468251000
B	8.025988000	10.075349000	10.016176000
B	9.372496000	11.160719000	9.504412000
B	8.798049000	8.253265000	9.907168000
B	10.512334000	9.229016000	8.005710000
B	10.256032000	7.750733000	10.767831000
B	12.224492000	8.530817000	8.715712000

Table SVIII. Cartesian coordinates of the lowest-energy structure of RuB_{24}.

Ru	9.797332000	9.729665000	9.782316000
B	9.155739000	11.402946000	11.155041000
B	9.658281000	7.510135000	9.811715000
B	7.545870000	9.418196000	9.568194000
B	12.026670000	9.206495000	9.746038000
B	9.719144000	8.645921000	7.703689000
B	9.582826000	10.978163000	12.712911000
B	9.840544000	8.130423000	11.438197000
B	7.858001000	9.818532000	11.234681000
B	11.671371000	10.462297000	10.927781000
B	10.658496000	10.246152000	13.853417000
B	8.112906000	9.826341000	12.851292000
B	11.364319000	10.402127000	12.537003000
B	9.059351000	9.985253000	14.008142000
B	11.744874000	10.723829000	9.238340000
B	8.330692000	8.218568000	10.475809000
B	7.899230000	10.993461000	9.979551000
B	11.148494000	7.945089000	10.354401000
B	9.889679000	9.078364000	12.805672000
B	10.002740000	10.204215000	7.549959000
B	8.420252000	8.289411000	8.721703000
B	10.689890000	11.704758000	10.114987000
B	10.987247000	8.204491000	8.701665000
B	9.158718000	11.899319000	9.472767000
B	10.421698000	11.468565000	8.423452000

Table SIX. Cartesian coordinates of the lowest-energy structure of OsB_{24}.

Os	9.750767000	10.076586000	9.624720000
B	9.913387000	9.506367000	7.449027000
B	10.221785000	9.819635000	13.446282000
B	10.480556000	12.025361000	10.686569000
B	9.692301000	7.531488000	10.010888000
B	7.441714000	9.709129000	9.558241000
B	12.025869000	9.472033000	9.670346000
B	10.788465000	10.980399000	7.835220000
B	8.321265000	9.410827000	8.099598000
B	9.069891000	10.968781000	7.598871000
B	11.373326000	9.372455000	8.113265000
B	10.612359000	8.383200000	12.808849000
B	9.215470000	10.870405000	12.987192000
B	10.574587000	10.750571000	11.912497000
B	9.102741000	9.167933000	12.254593000
B	11.048163000	8.179008000	9.341891000
B	7.927354000	11.127769000	8.700965000
B	10.971033000	11.886029000	9.187454000
B	8.341802000	8.295798000	9.425591000
B	11.663857000	10.698822000	10.693070000
B	8.055024000	9.379453000	10.984796000
B	7.904302000	11.154086000	10.364696000
B	11.157708000	9.005095000	11.093150000
B	10.038471000	7.594512000	11.648238000
B	8.986533000	11.701539000	11.561346000

Table SX. Cartesian coordinates of isomer I of WB_{24} in Fig. 3.

W	9.592424560	9.779479600	9.526255760
B	8.132035392	9.920824442	7.474716873
B	8.574249422	8.349222196	7.683771356
B	10.209243325	8.405971041	7.502759889
B	11.348349478	9.578429303	7.695034284
B	10.482655741	10.962387176	7.484260461
B	8.896918882	11.366193502	7.661939135
B	8.100928206	9.953661869	11.552736911
B	8.546086687	8.378951396	11.375786359
B	10.178136139	8.438808468	11.580779927
B	11.320186743	9.608158503	11.387049288
B	10.451548556	10.995224603	11.562280499
B	8.868756148	11.395922702	11.353954138
B	7.601345164	10.928877878	10.320688253
B	7.404527243	9.088623089	10.334005201
B	9.588788566	7.495698450	10.363493474
B	11.280899758	8.245474976	10.370363496
B	11.568403073	10.933641530	10.350910660
B	10.073109802	12.024119793	10.330723691
B	7.417018494	9.075437050	8.696455130
B	9.601279818	7.482512412	8.725943403
B	11.293391010	8.232288938	8.732813424
B	11.580894325	10.920455491	8.713360588
B	10.085601053	12.010933754	8.693173619
B	7.613836415	10.915691839	8.683138182

Table SXI. Cartesian coordinates of isomer II of WB_{24} in Fig. 3.

W	9.592424120	9.779479480	9.526256240
B	7.866011380	9.950478261	7.656871213
B	8.757642161	8.596638068	7.498267342
B	10.316081080	8.163770830	7.690459935
B	11.043599514	9.609598010	7.507854902
B	10.638518419	11.179039488	7.668499417
B	9.023494689	11.082754592	7.480160694
B	8.141248726	9.949360950	11.544657578
B	8.546329821	8.379919472	11.384013063
B	10.161353551	8.476204368	11.572351786
B	11.318836860	9.608480699	11.395641267
B	10.427206079	10.962320892	11.554245138
B	8.868767160	11.395188130	11.362052545
B	7.611988247	10.924040885	10.294230559
B	7.415942459	9.090721200	10.307582818
B	9.587621010	7.507029843	10.337354995
B	11.273338705	8.254009876	10.344425084
B	11.559138841	10.926666198	10.324959847
B	10.069466934	12.013005850	10.304537499
B	7.625709399	8.632292762	8.727552633
B	9.115381306	7.545953110	8.747974981
B	11.572859993	8.634918075	8.758281921
B	11.768905781	10.468237760	8.744929662
B	9.597227230	12.051929117	8.715157485
B	7.911509535	11.304949084	8.708087396

Table SXII. Cartesian coordinates of isomer III of WB_{24} in Fig. 3.

W	9.910210000	10.015341000	9.521081000
B	10.256775000	7.958276000	10.760761000
B	12.039083000	9.684497000	10.643806000
B	11.025651000	11.946066000	10.478259000
B	7.521665000	10.515738000	10.084811000
B	8.698059000	7.969673000	10.134706000
B	10.973723000	12.206291000	8.851454000
B	8.254181000	11.768769000	9.044527000
B	7.711244000	8.951815000	9.244007000
B	10.069656000	7.517185000	9.183662000
B	12.304494000	9.518959000	9.031998000
B	10.457793000	11.248075000	7.514220000
B	8.838022000	10.983861000	7.538129000
B	8.504174000	9.252407000	7.660726000
B	9.910017000	8.407069000	7.715526000
B	11.228532000	9.625889000	7.611992000
B	10.881257000	9.134352000	11.689819000
B	11.194744000	10.760415000	11.574690000
B	9.666791000	11.590423000	11.400914000
B	8.431991000	10.438704000	11.475269000
B	9.150716000	8.913180000	11.590657000
B	11.363842000	8.244965000	8.572801000
B	11.890255000	10.975443000	8.379503000
B	9.557449000	12.427255000	9.819046000
B	7.623951000	10.381218000	8.463466000

Table SXIII. Cartesian coordinates of isomer IV of WB_{24} in Fig. 3.

W	9.840052000	9.873606000	10.088767000
B	8.958811000	12.166182000	9.745022000
B	7.464491000	9.874719000	9.617500000
B	9.244947000	7.615208000	9.518478000
B	11.791110000	8.592863000	9.512603000
B	11.602643000	11.463422000	9.608192000
B	9.181668000	11.597381000	11.596692000
B	7.662682000	9.897298000	11.313588000
B	9.377682000	7.714320000	11.219434000
B	11.633154000	8.580387000	11.214195000
B	11.446641000	11.350276000	11.305127000
B	9.706488000	10.235487000	12.497388000
B	9.784904000	10.002369000	7.579810000
B	7.773492000	11.305402000	10.569315000
B	8.002785000	8.442537000	10.526641000
B	10.739579000	7.532193000	10.353244000
B	12.164596000	10.040501000	10.517338000
B	10.419045000	12.321087000	10.563156000
B	9.382013000	8.516031000	8.147249000
B	11.081361000	9.168606000	8.143277000
B	10.970912000	10.939554000	8.189346000
B	9.248888000	11.402657000	8.263759000
B	8.278972000	9.906001000	8.195482000
B	8.702366000	8.890496000	12.114661000
B	11.351223000	9.907550000	12.108746000

Table SXIV. Cartesian coordinates of isomer V of WB_{24} in Fig. 3.

W	9.779607000	9.724186000	9.941775000
B	10.865407000	9.082490000	12.059703000
B	8.693808000	10.365885000	7.823848000
B	9.847719000	9.255009000	7.522656000
B	9.711494000	10.193364000	12.360896000
B	11.982539000	8.914805000	9.416893000
B	7.576675000	10.533569000	10.466659000
B	8.854961000	11.924940000	10.232904000
B	10.704254000	7.523434000	9.650647000
B	8.382114000	7.968953000	11.060501000
B	11.177100000	11.479421000	8.823050000
B	7.528257000	9.594664000	8.985503000
B	12.030957000	9.853710000	10.898049000
B	11.409629000	9.959012000	8.128731000
B	8.149584000	9.489362000	11.754821000
B	10.148609000	11.665258000	11.389272000
B	9.410606000	7.783114000	8.494280000
B	11.548910000	11.416338000	10.481104000
B	8.010304000	8.032036000	9.402448000
B	11.552645000	8.255290000	10.893060000
B	8.006569000	11.193083000	8.990492000
B	10.031844000	7.677775000	11.263666000
B	9.527369000	11.770599000	8.619885000
B	10.953402000	8.356869000	8.221647000
B	8.605813000	11.091505000	11.661905000

Table SXV. Cartesian coordinates of isomer VI of WB_{24} in Fig. 3.

W	0.009729000	-0.020817000	0.008156000
B	0.059839000	-2.303367000	0.941327000
B	-0.359435000	-2.333816000	-0.666870000
B	2.566277000	-0.907260000	-0.846843000
B	-0.081566000	-1.508624000	-2.104612000
B	1.431524000	-1.551543000	-1.642469000
B	2.526064000	0.402583000	0.168507000
B	1.515622000	1.711730000	-0.412058000
B	1.934010000	0.447664000	-1.496446000
B	1.923215000	0.036016000	1.687024000
B	1.266573000	-1.439019000	1.550578000
B	-1.022047000	-1.333819000	1.881565000
B	0.666098000	1.038951000	2.115616000
B	-0.922861000	1.549597000	1.675129000
B	-0.810248000	0.149323000	2.420915000
B	0.386750000	2.173777000	0.834003000
B	-1.588981000	-1.371589000	-1.295526000
B	-1.522290000	-1.747206000	0.410958000
B	-2.049597000	-0.091256000	1.238934000
B	-2.377944000	0.895020000	-0.056996000
B	-1.259996000	2.198572000	0.190761000
B	-0.007928000	2.357743000	-0.826078000
B	-0.725967000	0.152437000	-2.317483000
B	-2.148838000	0.184050000	-1.516732000
B	0.591986000	1.310853000	-1.941390000

Table SXVI. Cartesian coordinates of isomer VII of WB_{24} in Fig. 3.

W	10.814921000	9.884273000	8.779261000
B	12.957968000	9.238864000	8.955828000
B	11.896815000	11.991808000	8.587871000
B	7.979767000	10.651865000	8.470462000
B	8.172205000	9.007319000	8.981701000
B	9.399603000	8.296811000	8.041503000
B	10.267308000	8.988140000	12.195884000
B	8.678990000	9.640374000	7.533081000
B	10.702042000	10.085525000	10.901442000
B	9.968493000	8.492807000	10.566055000
B	11.762045000	9.120189000	11.828116000
B	10.157331000	11.651820000	10.730761000
B	8.553503000	11.238546000	11.068915000
B	8.800382000	9.526316000	11.661954000
B	10.524664000	7.586978000	9.099471000
B	12.476023000	9.881122000	10.533910000
B	10.519099000	12.389840000	9.163013000
B	7.507634000	11.510809000	9.799064000
B	7.986482000	8.390719000	10.538781000
B	8.926741000	7.526652000	9.548537000
B	12.089684000	7.963359000	8.993951000
B	11.722026000	11.482094000	10.293221000
B	8.942638000	12.226819000	9.744833000
B	7.588369000	9.968928000	10.362700000
B	12.888568000	10.843568000	9.071090000