

Supporting Information

Insights into ThB₄₀: Stability, Electronic Structure, and Interaction

Yutian Li ^{1,*}, Yingying Wang ¹, Zhanrong Zhou ¹, Yang Gao ¹, Yiming Chen ¹, Guoqing Zhang ¹ and Chao Ma ²

¹ Xi'an Research Institute of High Technology, Xi'an 710025, China;
gaoyang_nudt@126.com (Y.G.)

² Foundation Department, Engineering University of PAP, Xi'an
710086, China

* Correspondence: lyt13593587864@stu.xjtu.edu.cn

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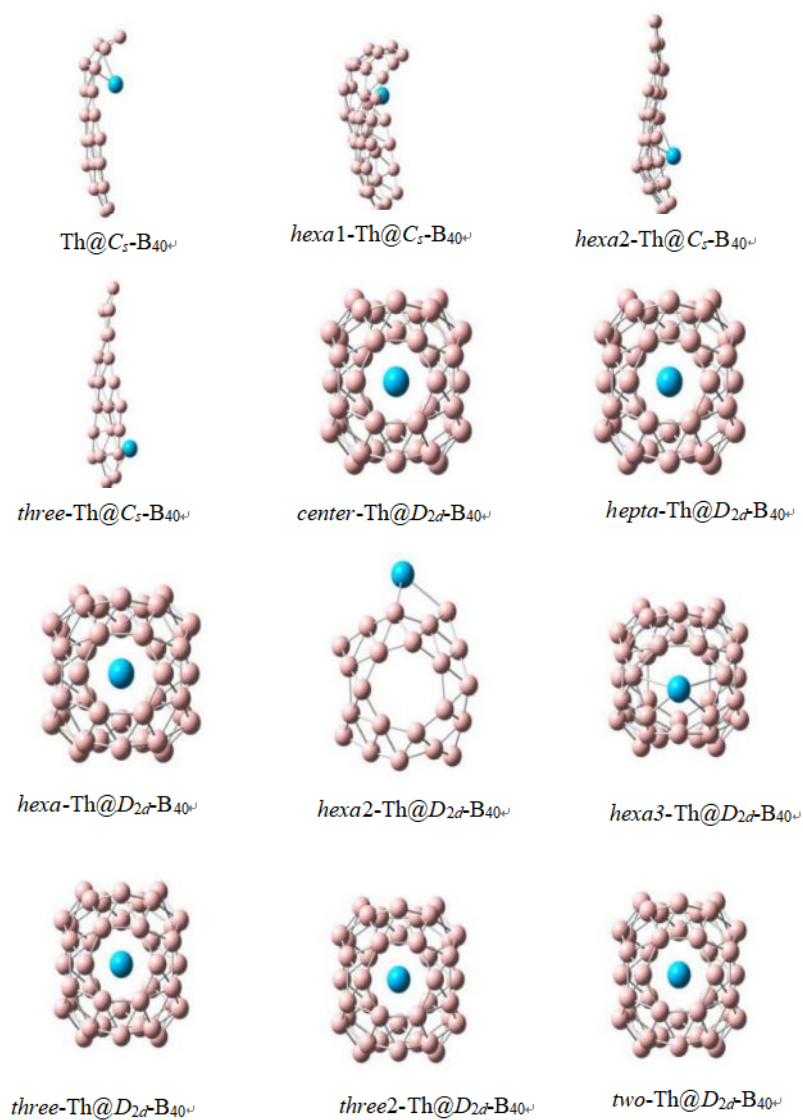


Figure S1 Potential isomers of ThB₄₀ based on D_{2d}-B₄₀ and C₅-B₄₀ isomers optimized on the TPSSH/6-31G*~SDD. The Th atoms are colored in blue and B atoms are colored in pink.

Table S1 Relative energy of D_{2d} -B₄₀ and C_s -B₄₀ in different spin multiplicities optimized on the the TPSSH/6-31G* theoretical level.

| Isomers | Singlet/a.u. | Triplet/a.u. | $\Delta E/\text{kcal}\cdot\text{mol}^{-1}$ |
|---------------------------|--------------|--------------|--|
| D_{2d} -B ₄₀ | -994.035351 | -993.970392 | 40.8 |
| C_s -B ₄₀ | -994.011059 | -993.998578 | 7.8 |

Table S2 Relative energy ($\text{kcal}\cdot\text{mol}^{-1}$) of Th@ D_{2d} -B₄₀ and Th@ C_s -B₄₀ at different functionals with 6-31G*~SDD basis set.

| Isomers | B3LYP | BP86 | PBE0 | HSE06 |
|-------------------------------|-------|------|------|-------|
| Th@ D_{2d} -B ₄₀ | 0.0 | 0.0 | 0.0 | 0.0 |
| Th@ C_s -B ₄₀ | 29.2 | 60.5 | 65.0 | 61.3 |

Table S3 Relative energy ($\text{kcal}\cdot\text{mol}^{-1}$) of Th@ D_{2d} -B₄₀ in different spin multiplicities optimized on the different functionals with 6-31G*~SDD basis set.

| Isomers | B3LYP | BP86 | PBE0 | HSE06 |
|---------|-------|------|------|-------|
| Singlet | 0.0 | 0.0 | 0.0 | 0.0 |
| Triplet | 1.7 | 1.8 | 1.0 | 1.0 |

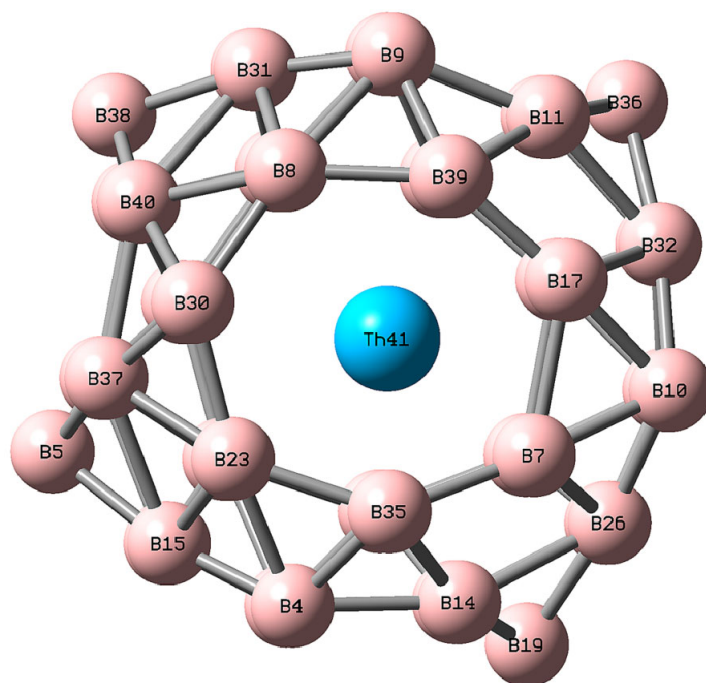


Figure S2 Geometry of Th@ D_{2d} -B₄₀ with atom labels.

Table S4 Parameters of bond critical points between B and Th atoms.

| | P_{BCP} | $\nabla^2 \rho_{BCP}$ | G_{BCP}/ρ_{BCP} | H_{BCP}/ρ_{BCP} | $ V_{BCP} /\rho_{BCP}$ |
|--------|-----------|-----------------------|----------------------|----------------------|------------------------|
| Th-B7 | 0.033 | 0.055 | 0.566 | -0.147 | 0.713 |
| Th-B8 | 0.025 | 0.052 | 0.602 | -0.090 | 0.692 |
| Th-B15 | 0.026 | 0.044 | 0.520 | -0.094 | 0.614 |
| Th-B17 | 0.033 | 0.055 | 0.566 | -0.147 | 0.713 |
| Th-B32 | 0.031 | 0.054 | 0.560 | -0.120 | 0.680 |

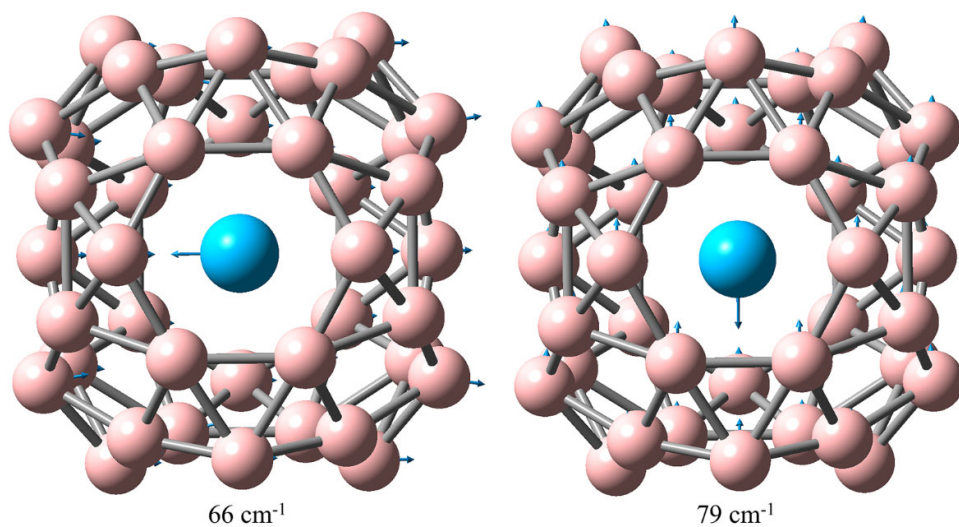


Figure S3 Maps of feature displacement vectors in Th@D_{2d}-B₄₀ simulated on the TPSSh/6-31G*~SDD. The Th atoms are colored in blue and B atoms are colored in pink. The vectors are marked by blue arrows.

Coordinates of D_{2d} -B₄₀, C_s -B₄₀, Th@ D_{2d} -B₄₀, and Th C_s -B₄₀

D_{2d} -B₄₀

| | | | |
|---|-------------|-------------|-------------|
| B | 1.75260100 | 2.74276900 | -0.38394100 |
| B | 1.69437100 | 0.00000000 | 2.87638700 |
| B | 1.39005000 | 2.37032000 | 1.20490500 |
| B | -1.75260500 | -2.74277100 | -0.38394100 |
| B | 0.00000100 | -1.69437400 | -2.87638600 |
| B | 2.65161400 | 0.00000100 | -1.99487700 |
| B | -2.37185900 | -0.87949400 | 1.68046200 |
| B | -2.37031700 | 1.39004900 | -1.20490700 |
| B | -1.75260400 | 2.74277100 | -0.38394500 |
| B | -1.69437000 | 0.00000100 | 2.87638600 |
| B | -1.39004900 | 2.37031900 | 1.20490100 |
| B | 2.74277000 | -1.75259000 | 0.38394200 |
| B | 1.39005400 | -2.37031900 | 1.20490800 |
| B | -1.39005100 | -2.37031900 | 1.20490400 |
| B | -0.87948800 | -2.37184400 | -1.68044200 |
| B | 0.87948800 | 2.37184400 | -1.68044900 |
| B | -2.37185600 | 0.87949500 | 1.68045800 |
| B | 0.87949800 | -2.37185700 | -1.68046100 |
| B | 0.00000000 | -2.65161400 | 1.99486400 |
| B | 2.74277000 | 1.75259100 | 0.38394300 |
| B | 2.37185800 | 0.87949500 | 1.68046200 |
| B | 2.37185100 | -0.87949600 | 1.68045900 |
| B | -2.37032000 | -1.39004900 | -1.20490400 |
| B | 2.37031500 | 1.39004900 | -1.20490400 |
| B | 2.37032400 | -1.39004800 | -1.20490700 |
| B | -0.88977100 | -1.39150500 | 2.54058300 |
| B | 0.88976900 | -1.39150600 | 2.54058900 |
| B | 1.75259700 | -2.74276600 | -0.38394200 |
| B | 1.39150100 | -0.88976700 | -2.54058100 |
| B | -2.65161100 | 0.00000000 | -1.99487600 |
| B | -0.87949000 | 2.37184500 | -1.68045300 |
| B | -0.88977000 | 1.39150600 | 2.54058200 |

C_s -B₄₀

| | | | |
|---|-------------|-------------|------------|
| B | -0.38248100 | 2.17586700 | 1.71409600 |
| B | 0.09764200 | 2.15632900 | 3.36305000 |
| B | 0.23227700 | 0.73390000 | 4.19430100 |
| B | -0.23130500 | -0.71027900 | 3.33041300 |
| B | -0.69718300 | -0.70405000 | 1.65693800 |
| B | -0.75186600 | 0.74848000 | 0.82571100 |

| | | | |
|---|-------------|-------------|-------------|
| B | -0.67252300 | -2.16161100 | 0.82965500 |
| B | 0.36686500 | -2.11286500 | 4.12071900 |
| B | 0.19624400 | 3.46064000 | 0.84034600 |
| B | -0.29084600 | -2.12673000 | 2.47346200 |
| B | 0.22324500 | 3.54168300 | 2.54492300 |
| B | 0.50418700 | -0.68845900 | 4.81932600 |
| B | 0.41668700 | -3.55737000 | 3.28810400 |
| B | -0.13570900 | -3.57567800 | 1.65830800 |
| B | 0.42471500 | -4.98658300 | 0.82813100 |
| B | -0.69717300 | -0.70404800 | -1.65693600 |
| B | -0.29084100 | -2.12673000 | -2.47345600 |
| B | -0.13578300 | -3.57569400 | -1.65831400 |
| B | 0.42470900 | -4.98657900 | -0.82814100 |
| B | 0.65049000 | -4.84008600 | -2.39369700 |
| B | 0.41651300 | -3.55742700 | -3.28814800 |
| B | 0.36698800 | -2.11285500 | -4.12066700 |
| B | -0.23126800 | -0.71028100 | -3.33040500 |
| B | 0.50430500 | -0.68845200 | -4.81927900 |
| B | 0.09763800 | 2.15632800 | -3.36305000 |
| B | 0.23224800 | 0.73390800 | -4.19432000 |
| B | -0.38247000 | 2.17586300 | -1.71409300 |
| B | 0.22327200 | 3.54167600 | -2.54491700 |
| B | 0.19625000 | 3.46063900 | -0.84034300 |
| B | -0.47971100 | 0.76066200 | -2.49335000 |
| B | -0.47971200 | 0.76066300 | 2.49334800 |
| B | -0.30456500 | -3.59595800 | 0.00000100 |
| B | -0.75187000 | 0.74847900 | -0.82571200 |
| B | 0.65068900 | -4.84002100 | 2.39365100 |
| B | 0.26565800 | 4.96766000 | 1.71314800 |
| B | -0.09146000 | 4.89717300 | -0.00000100 |
| B | 0.26567300 | 4.96765700 | -1.71314800 |
| B | 0.46150700 | 6.26788100 | -0.78390100 |
| B | 0.46150500 | 6.26788100 | 0.78390000 |
| B | -0.67253700 | -2.16161300 | -0.82965400 |

Th@D_{2d}-B₄₀

| | | | |
|---|-------------|-------------|-------------|
| B | 1.66177800 | 2.77627300 | -0.36578500 |
| B | 1.60870000 | 0.00074000 | 2.93216200 |
| B | 1.36858700 | 2.44459100 | 1.25574500 |
| B | -1.70480900 | -2.77450100 | -0.36486800 |
| B | -0.02229600 | -1.69473500 | -2.94504400 |
| B | 2.53853100 | 0.00048700 | -1.89295200 |
| B | -2.32762700 | -0.88028600 | 1.70746400 |

| | | | |
|----|-------------|-------------|-------------|
| B | -2.34809700 | 1.45357400 | -1.21866200 |
| B | -1.70464800 | 2.77612700 | -0.36518000 |
| B | -1.65362700 | 0.00093500 | 2.93325400 |
| B | -1.41344200 | 2.44513100 | 1.25691500 |
| B | 2.61450500 | -1.68626900 | 0.39450300 |
| B | 1.36836900 | -2.44327700 | 1.25601500 |
| B | -1.41389000 | -2.44331700 | 1.25726900 |
| B | -0.87062300 | -2.38460200 | -1.66639800 |
| B | 0.82696500 | 2.38565100 | -1.66717000 |
| B | -2.32761600 | 0.88183700 | 1.70725800 |
| B | 0.82674900 | -2.38451300 | -1.66693900 |
| B | -0.02241100 | -2.73137900 | 2.01704600 |
| B | 2.61461700 | 1.68737900 | 0.39427400 |
| B | 2.28390000 | 0.88166100 | 1.70696300 |
| B | 2.28395600 | -0.88041700 | 1.70717000 |
| B | -2.34830700 | -1.45209500 | -1.21857600 |
| B | 2.30436400 | 1.45348800 | -1.21898600 |
| B | 2.30431800 | -1.45240200 | -1.21880000 |
| B | -0.87584600 | -1.39955900 | 2.58826500 |
| B | 0.83207100 | -1.40068300 | 2.58793100 |
| B | 1.66151000 | -2.77501800 | -0.36551200 |
| B | 1.33017300 | -0.88573900 | -2.57784600 |
| B | -2.58256300 | 0.00073200 | -1.89309300 |
| B | -0.87039000 | 2.38592100 | -1.66662200 |
| B | -0.87571700 | 1.40126100 | 2.58793800 |
| B | 0.83225100 | 1.40224900 | 2.58785800 |
| B | 1.33020800 | 0.88670900 | -2.57791500 |
| B | -2.65854800 | -1.68591700 | 0.39463300 |
| B | -0.02210100 | 2.73297800 | 2.01693200 |
| B | -1.37481100 | -0.88598700 | -2.57796700 |
| B | -0.02214600 | 1.69587700 | -2.94521400 |
| B | -2.65831800 | 1.68764400 | 0.39451400 |
| B | -1.37471300 | 0.88724400 | -2.57805200 |
| Th | -0.02260900 | 0.00062100 | 0.11119300 |

ThC₅-B₄₀

| | | | |
|---|-------------|-------------|------------|
| B | -0.33628900 | 1.90723400 | 1.62408600 |
| B | 0.41432400 | 1.71381300 | 3.20409900 |
| B | 0.11321800 | 0.43842300 | 4.17044400 |
| B | -0.57326900 | -0.92232900 | 3.32651700 |
| B | -1.03296100 | -0.86951500 | 1.67471600 |
| B | -1.09236600 | 0.59868700 | 0.85839700 |
| B | -0.94851500 | -2.27884600 | 0.80754700 |

| | | | |
|----|-------------|-------------|-------------|
| B | -0.23068800 | -2.38789300 | 4.16082100 |
| B | -0.26419100 | 3.46578600 | 0.96415400 |
| B | -0.84756900 | -2.34710400 | 2.50525600 |
| B | 0.86640400 | 2.95686700 | 2.28118800 |
| B | 0.08835900 | -0.98014200 | 4.86169500 |
| B | -0.08803900 | -3.76445500 | 3.29375900 |
| B | -0.38289300 | -3.68232800 | 1.57662000 |
| B | 0.56248100 | -4.85929400 | 0.76493200 |
| B | -1.13940100 | -0.60270300 | -1.57730400 |
| B | 0.37872500 | -1.41082700 | -1.93871100 |
| B | 0.44108600 | -3.08528500 | -1.55196100 |
| B | 1.11014700 | -4.46101600 | -0.74076100 |
| B | 1.87043500 | -3.84426200 | -1.96264800 |
| B | 1.63423500 | -2.44915000 | -2.67228100 |
| B | 1.37349600 | -0.95924900 | -3.26476600 |
| B | -0.21103200 | -0.20859600 | -2.98534900 |
| B | 1.04015300 | 0.45662000 | -3.90519900 |
| B | -1.27378800 | 2.38971100 | -3.04070400 |
| B | -0.17541300 | 1.42536400 | -3.69626000 |
| B | -1.80177700 | 2.26562700 | -1.40221900 |
| B | -1.33600400 | 3.70598100 | -2.12042600 |
| B | -1.01145000 | 3.73789500 | -0.44772200 |
| B | -1.44470700 | 0.86120700 | -2.34460600 |
| B | -0.66873100 | 0.56399800 | 2.52219800 |
| B | -0.25217600 | -3.52898600 | -0.07908800 |
| B | -1.70300100 | 0.79196900 | -0.65795100 |
| B | 0.44397200 | -4.91057400 | 2.34506500 |
| B | 1.59947200 | 3.78431400 | 1.13120400 |
| B | 0.57271900 | 4.43734000 | -0.15247400 |
| B | -0.05719100 | 4.58917500 | -1.73759500 |
| B | 1.51361200 | 4.74446300 | -1.51349000 |
| B | 2.26308000 | 4.28375600 | -0.23126100 |
| B | -0.76784300 | -2.07319400 | -0.84529000 |
| Th | 0.81486900 | 1.87567200 | -1.07554100 |