

Supporting Information
Of
H©Be₄S₄⁻: A Superhalogen Planar Tetracoordinate Hydrogen Cluster

Table S1. Lowest vibrational frequencies (cm^{-1}) at different theoretical levels for the global minimum D_{4h} ptH cluster.

Theoretical level	Lowest vibrational frequency (cm^{-1})
B2PLYP-D3(BJ)/def2-TZVP	60.3
M06-L/ def2-TZVP	59.7
MP2/ def2-TZVP	61.9
TPSS-D3(BJ)/def2-TZVP	58.8
ω B97XD/def2-TZVP	61.7
PBE0/def2-TZVP	62.0

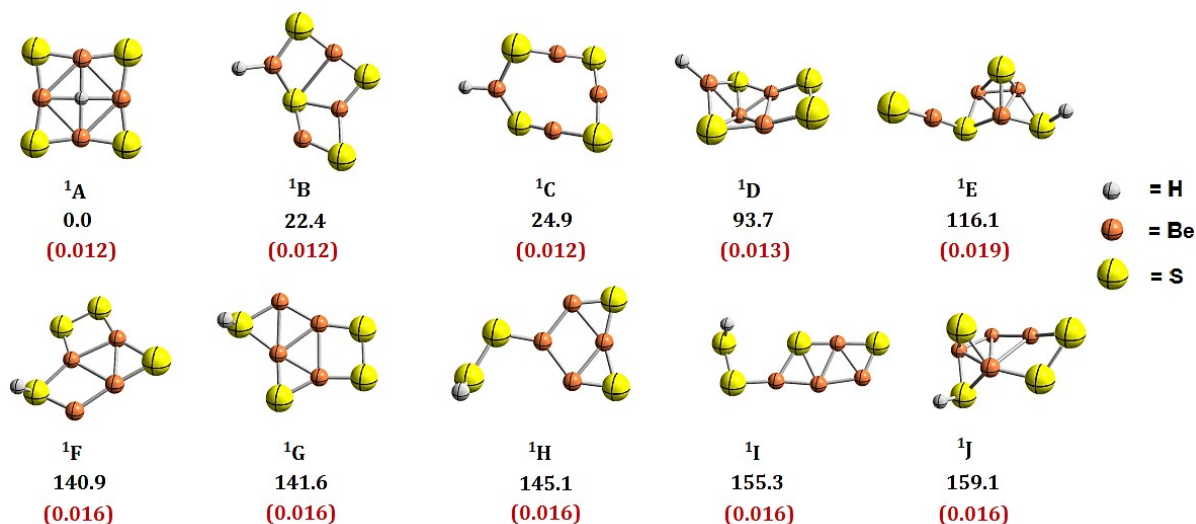
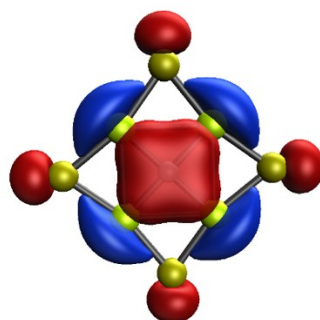


Fig S1. Relative energies (kcal/mol) of the isomers calculated at CCSD(T)/aug-cc-pVTZ//M06-2X/def2-TZVP level. T_1 diagnostic values are shown in red font and within parenthesis.



$$\Delta E_{\text{orb}} = -128.9$$

$$|\nu| = 0.79$$

Fig S2. The shapes of deformation densities ($\Delta\rho$) for ETS-NOCV analysis of $\text{H}\text{©}\text{Be}_4\text{S}_4^-$ cluster. Direction of charge flow is from red to blue and energy is in kcal/mol.

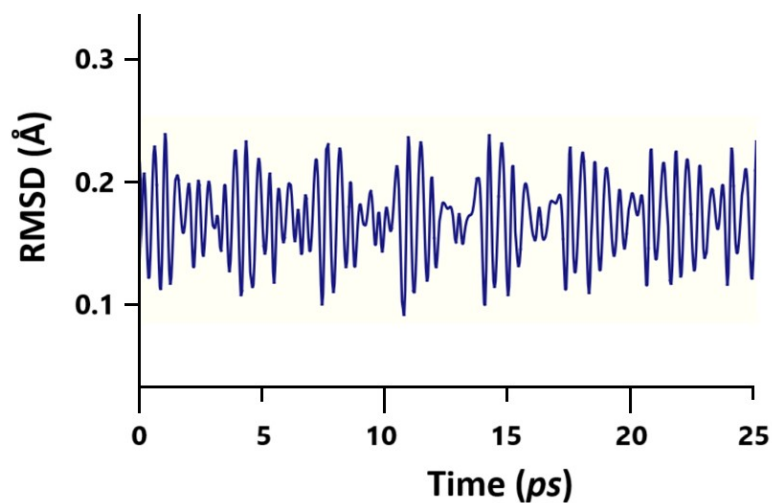


Fig S3. Root-mean square deviation, RMSD (Å) versus time plot obtained using Born-Oppenheimer molecular dynamics (BOMD) simulation at 298K calculated at M06-2X/def2-TZVP level for a time period of 25 ps.

Cartesian coordinates of the optimized geometries shown in Fig S1 at M06-2X/def2-TZVP level.

Bare neutral Be₄S₄

4	-0.855770000	-1.728178000	0.000000000
4	-1.729194000	0.856272000	0.000000000
4	1.729212000	-0.856281000	0.000000000
4	0.855771000	1.728183000	0.000000000
16	-2.534616000	-0.855732000	0.000000000
16	-0.855770000	2.534602000	0.000000000
16	2.534610000	0.855728000	0.000000000
16	0.855771000	-2.534597000	0.000000000

¹A

4	-1.591847000	0.449743000	0.000000000
4	0.447373000	1.586003000	0.000000000
4	-0.449147000	-1.591285000	0.000000000
4	1.593473000	-0.449053000	0.000000000
1	0.000000000	0.000810000	0.000000000
16	-1.322711000	2.363757000	0.000000000
16	2.363256000	1.323484000	0.000000000
16	1.322985000	-2.363343000	0.000000000
16	-2.363494000	-1.322800000	0.000000000

¹B

4	1.214236000	-0.217275000	1.321627000
4	-0.910952000	1.116162000	0.785003000
4	0.815014000	2.943340000	-0.294259000
4	3.106355000	0.493363000	0.665415000

16	-1.160552000	2.709699000	-0.192871000
16	-0.686652000	-0.580357000	1.612042000
16	1.926820000	1.866194000	1.195999000
16	2.871747000	-1.330438000	0.854582000
1	1.549389000	3.761987000	-1.097987000

¹³C

4	-0.077519000	2.064047000	0.195354000
4	0.767351000	-0.302884000	0.721523000
4	1.735124000	3.958794000	1.823494000
4	2.424579000	0.969911000	2.203067000
16	2.161109000	2.495943000	3.211772000
16	-0.946787000	0.338709000	0.261678000
16	2.535575000	-0.705164000	1.245758000
16	0.866321000	3.639566000	-0.015991000
1	2.052180000	5.249679000	2.153564000

¹³D

4	2.606663000	0.400400000	0.724134000
4	1.725152000	2.277450000	1.330168000
4	-0.349607000	0.503805000	-0.050291000
4	1.517781000	1.526315000	-0.495598000
16	-0.016370000	2.564530000	0.242594000
16	2.525404000	2.070491000	3.113528000
16	1.402043000	-0.450071000	-0.733524000
16	3.395418000	0.206041000	2.513976000
1	-1.565532000	-0.085043000	0.000252000

¹E

4	2.168920000	0.434991000	2.550846000
4	3.741487000	-1.889247000	1.624243000
4	0.816237000	1.693569000	1.172251000
4	2.006762000	0.341313000	0.309742000
16	0.525096000	-0.276178000	1.711877000
16	1.672370000	2.424283000	3.007298000
16	3.831964000	-3.653372000	1.873757000
16	3.764060000	0.106864000	1.357096000
1	0.617206000	2.038674000	3.746296000

¹F

4	1.737045000	1.878149000	0.617853000
4	0.084648000	0.348547000	0.130508000
4	2.040885000	-0.407168000	0.386153000
4	-0.560207000	2.244315000	0.283827000
16	3.639711000	1.965884000	1.000329000
16	3.951439000	-0.124928000	0.782569000
16	0.675981000	3.824661000	0.714660000
16	0.520649000	-1.524916000	-0.012614000
1	0.433942000	3.685538000	2.028141000

¹G

4	1.178548000	-0.295833000	1.328133000
4	0.247269000	1.425694000	0.608039000
4	1.579152000	3.023505000	-0.460802000

4	2.469924000	1.325184000	0.200599000
16	-0.453472000	3.312410000	-0.182907000
16	2.770585000	-1.412926000	1.561806000
16	-0.714735000	0.079051000	1.581172000
16	3.918688000	0.087930000	0.580787000
1	-0.228123000	3.936569000	0.984315000

¹H

4	1.992838000	0.385988000	1.089769000
4	1.393875000	1.459533000	-0.608612000
4	0.543769000	0.786216000	2.569733000
4	-0.165359000	1.944501000	0.850014000
16	-1.021986000	1.839616000	2.617698000
16	-0.059530000	2.597198000	-1.002321000
16	4.791033000	-0.972196000	-0.072283000
16	3.497818000	-0.760794000	1.583379000
1	5.377177000	0.229725000	-0.003595000

¹H

4	-0.044652000	1.420547000	0.669534000
4	1.452935000	-0.160898000	0.251425000
4	-0.627728000	-0.480464000	0.288352000
4	3.322079000	0.551205000	0.317032000
16	1.769864000	1.953963000	0.690678000
16	5.348655000	3.035899000	0.842683000
16	-1.935101000	0.836980000	0.637240000
16	5.228081000	1.048800000	0.199904000

1	4.559903000	3.591196000	-0.087335000
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¹J

4	1.715996000	1.183600000	-1.236916000
4	-0.210282000	1.546618000	-0.528403000
4	-0.311157000	1.871958000	1.486467000
4	1.872212000	1.295078000	1.492357000
16	0.420714000	0.182330000	2.598607000
16	1.244500000	3.133624000	1.582226000
16	3.655999000	1.337380000	-1.338966000
16	3.008961000	0.141657000	0.287805000
1	0.795295000	0.880135000	3.684807000