Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Of

Planar pentacoordinate carbon in 16 electron neutral $CCu_2Be_4H_4$ cluster

Amlan J. Kalita,[a] Namrata Gohain,[a] Abhik Bordoloi,[a] and Ankur K. Guha*[a]

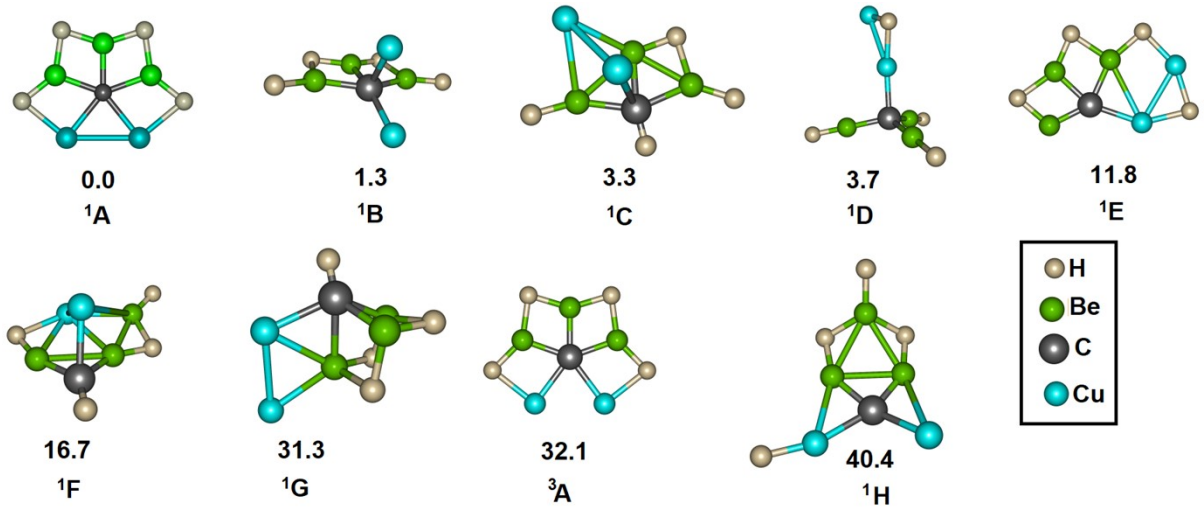

Fig S1. Relative energies (kcal/mol) of the low-lying energy isomers (**A-H**) of C $Cu_2Be_3H_4$ cluster computed at CCSD(T)/def2-TZVP//TPSSh/def2-TZVP level.

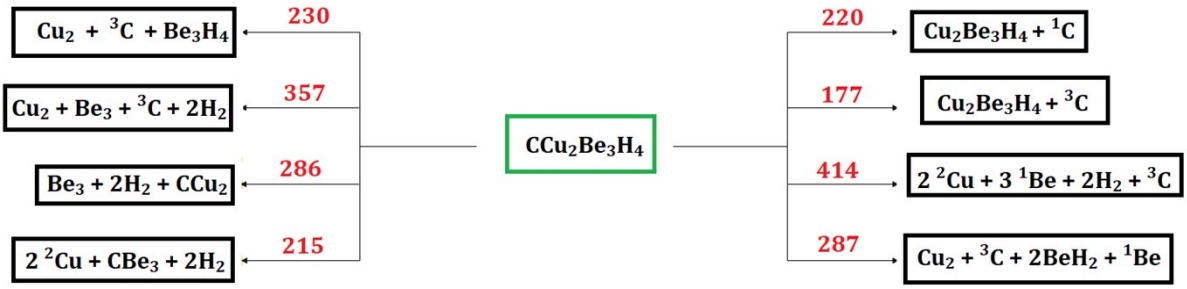

Fig S2. Different decomposition pathways and their energies (kcal/mol) including ZPE calculated at TPSSh/def2-TZVP level.

Table S1. HOMO-LUMO gap (ΔE_{H-L}, eV), Lowest vibrational frequency, ν_{min} (cm^{-1}), Wiberg bond index (WBI), and Mayer's bond order (MBO) in Lödwin orthogonalized bases of the global minimum planar cluster at different levels. In all calculations def2-TZVP basis set were used for all atoms.

Cluster	Functional	ΔE_{H-L} (eV)	ν_{min}	WBI		MBO	
				C-Cu	C-Be	C-Cu	C-Be
$CCu_2Be_3H_4$	M06-2X[1]	5.1	59	0.30	0.79	0.57	0.93
	ωB97XD[2]	3.7	80	0.37	0.76	0.63	0.89
	TPSSh[3]	2.5	92	0.41	0.74	0.62	0.87
	PBE0[4]	3.7	84	0.37	0.76	0.63	0.89

References

1. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc*., 2008, **120**, 215.

2. J. –D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.* 2008, **10**, 6615-6620.

3. J. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett*., 2003, **91**, 146401.

4. C. Adamo and V. Barone, *J. Chem. Phys*., 1999, **110**, 6158–6170.

Table S2. Electron density, ρ, at the bond critical point (bcp), Laplacian of electron density, $\nabla^2\rho$ and local electronic energy density, $H(r)$ calculated at TPSSh/def2-TZVP level. All values are in a. u.

Molecules	bcp	ρ	$\nabla^2\rho$	$H(r)$
$CCu_2Be_3H_4$	C-Cu	0.105	0.225	-0.045
	C-Be	0.086	0.406	-0.017

Cartesian coordinates of the optimized geometries and their total energies (in a. u.) at CCSD(T)/def2-TZVP//TPSSh/def2-TZVP.

^{1}A

Sum of electronic and zero-point Energies= -3365.849433

Sum of electronic and thermal Energies= -3365.841599

Sum of electronic and thermal Enthalpies= -3365.840655

Sum of electronic and thermal Free Energies= -3365.882380

$E_{CCSD(T)}$ = -3363.14262

6	0.000012000	0.918044000	0.000095000
29	1.219780000	-0.603284000	0.000433000
4	-1.605253000	1.497131000	0.001784000
1	-2.716731000	0.623844000	0.001876000
4	1.605291000	1.497149000	-0.001357000
1	1.391758000	3.004263000	-0.001120000
4	-0.000002000	2.562250000	-0.000300000
1	-1.391745000	3.004272000	0.000809000
29	-1.219785000	-0.603283000	-0.000472000
1	2.716668000	0.623684000	-0.001497000

^{1}B

Sum of electronic and zero-point Energies = **-3365.839494**

Sum of electronic and thermal Energies = **-3365.830543**

Sum of electronic and thermal Enthalpies = **-3365.829599**

Sum of electronic and thermal Free Energies = **-3365.875265**

$E_{CCSD(T)}$ = -3363.14054

29	-1.435370000	0.115214000	0.069540000
29	0.783206000	-1.039204000	-0.087427000

4	0.538674000	1.230155000	-1.610954000
4	1.619866000	1.826540000	-0.019447000
4	0.905582000	0.985003000	1.673097000
6	0.300888000	0.767180000	0.054890000
1	0.831926000	0.647496000	2.977444000
1	0.154021000	1.090402000	-2.897141000
1	2.086188000	2.038348000	1.291342000
1	1.778825000	2.249604000	-1.353065000

^{1}C

Sum of electronic and zero-point Energies = **-3365.844811**

Sum of electronic and thermal Energies = **-3365.836140**

Sum of electronic and thermal Enthalpies = **-3365.835196**

Sum of electronic and thermal Free Energies = **-3365.878351**

$E_{CCSD(T)}$ = -3363.13732

4	-0.016607000	0.365337000	1.605295000
4	-0.368010000	1.227908000	-0.366323000
29	-0.673689000	-0.952040000	-0.164130000
29	1.566560000	0.258503000	-0.137101000
4	-2.306891000	1.411544000	-0.620131000
1	-3.557850000	1.682478000	-1.033301000
1	-1.071532000	1.817742000	-1.459442000
1	0.768914000	-0.087262000	2.610245000
6	-1.487169000	0.677856000	0.781598000
1	-2.343742000	0.613342000	1.453230000

^{1}D

Sum of electronic and zero-point Energies = **-3365.830330**

Sum of electronic and thermal Energies = **-3365.820094**

Sum of electronic and thermal Enthalpies = **-3365.819150**

Sum of electronic and thermal Free Energies = **-3365.867538**

$E_{CCSD(T)}$ = -3363.13672

6	0.235144000	2.108522000	0.000000000
29	0.428395000	0.224021000	0.000000000
29	-0.595107000	-1.910142000	0.000000000
1	0.871962000	-1.339643000	0.000000000
4	1.734736000	2.725874000	0.000000000
1	2.965224000	3.254632000	0.000000000
4	-0.595107000	2.311579000	1.377986000
1	-1.295736000	2.467621000	2.510589000
4	-0.595107000	2.311579000	-1.377986000
1	-1.295736000	2.467621000	-2.510589000

^{1}E

Sum of electronic and zero-point Energies= **-3365.829763**

Sum of electronic and thermal Energies= **-3365.821747**

Sum of electronic and thermal Enthalpies= **-3365.820802**

Sum of electronic and thermal Free Energies= **-3365.863233**

$E_{CCSD(T)}$ = -3363.12414

4	3.256025000	-0.123208000	0.001472000
29	0.199278000	-1.038760000	-0.000191000
29	-1.533978000	0.472614000	0.000206000
4	0.556871000	1.364798000	-0.000591000
4	2.498410000	1.577539000	-0.000768000
6	1.705062000	0.106781000	-0.000523000
1	4.001417000	1.113354000	0.001506000
1	-1.500000000	-1.183004000	0.000871000

1	1.555380000	2.637273000	0.000249000
1	-0.826079000	1.933409000	-0.000378000

^{1}F

Sum of electronic and zero-point Energies = **-3365.829881**

Sum of electronic and thermal Energies = **-3365.821355**

Sum of electronic and thermal Enthalpies = **-3365.820411**

Sum of electronic and thermal Free Energies = **-3365.863586**

$E_{CCSD(T)}$ = -3363.11597

4	1.552048000	1.816063000	0.263631000
4	-0.009057000	0.850428000	1.206148000
4	-0.326629000	-1.426735000	0.842201000
29	1.317495000	-0.392742000	-0.159893000
1	0.546428000	2.175274000	1.324978000
1	2.377965000	2.757854000	-0.231126000
1	0.708839000	-2.098600000	0.170604000
29	-1.265529000	0.174579000	-0.554822000
6	-1.295742000	-0.218599000	1.380664000
1	-2.231236000	-0.155248000	1.930377000

^{1}G

Sum of electronic and zero-point Energies= **-3365.802610**

Sum of electronic and thermal Energies= **-3365.794772**

Sum of electronic and thermal Enthalpies= **-3365.793828**

Sum of electronic and thermal Free Energies= **-3365.835706**

$E_{CCSD(T)}$ = -3363.09276

4	-2.335843000	1.454967000	-0.755295000
4	-2.315985000	0.859543000	1.057465000
4	-0.522252000	1.020379000	-0.068253000

29	-0.222092000	-1.074368000	0.007957000
29	1.617952000	0.485021000	0.000180000
6	-1.987709000	-0.197806000	-0.140666000
1	-2.521870000	-0.812567000	-0.872227000
1	-1.126314000	2.159305000	-1.072908000
1	-3.144536000	1.990926000	0.348136000
1	-1.064651000	1.600676000	1.269373000

^{3}A

Sum of electronic and zero-point Energies= **-3365.793119**

Sum of electronic and thermal Energies= **-3365.785156**

Sum of electronic and thermal Enthalpies= **-3365.784212**

Sum of electronic and thermal Free Energies= **-3365.827098**

$E_{CCSD(T)}$ = -3363.09136

6	0.001690000	0.962157000	0.001713000
29	1.172626000	-0.614513000	0.001182000
4	-1.594152000	1.527353000	0.006389000
1	-2.606457000	0.511083000	0.001719000
4	1.597626000	1.525819000	-0.005051000
1	1.399638000	3.038368000	-0.003741000
4	0.002689000	2.625099000	-0.001002000
1	-1.393484000	3.039845000	-0.000064000
29	-1.174019000	-0.612371000	-0.001429000
1	2.605905000	0.504310000	-0.002382000

^{1}H

Sum of electronic and zero-point Energies= **-3365.783557**

Sum of electronic and thermal Energies= **-3365.774365**

Sum of electronic and thermal Enthalpies= **-3365.773421**

Sum of electronic and thermal Free Energies= **-3365.819809**

$E_{CCSD(T)}$ = -3363.07819

4	-0.854119000	1.588347000	-0.095876000
4	1.261175000	1.431376000	-0.609432000
29	1.477809000	-0.839506000	0.086321000
29	-1.583726000	-0.430102000	0.010806000
6	0.142331000	0.338599000	-0.330427000
4	0.527873000	3.295828000	0.313199000
1	-0.892983000	2.992684000	-0.029230000
1	1.622082000	2.776896000	-0.596019000
1	0.821057000	4.337470000	1.099904000
1	-3.072278000	-0.582213000	0.259668000