

Supporting Information available for

Identifying the Hydrogenated Planar Tetracoordinate Carbon: a Combined Experimental and Theoretical Study of CAI_4H and CAI_4H^-

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1. Experimental and theoretical methods

Anion photoelectron spectroscopy was conducted by crossing a mass-selected, negative ion beam with a fixed-energy photon beam and analyzing the energies of the resultant photodetached electrons. This technique is governed by the well-known energy-conserving relationship, $h\nu = EBE + EKE$, where $h\nu$, EBE , and EKE are the photon energy, electron binding energy (transition energy), and the electron kinetic energy, respectively. Our photoelectron instruments, which have been described elsewhere,¹ consist of an ion source, a linear time-of-flight mass spectrometer, a mass gate, a momentum decelerator, a neodymium-doped yttrium aluminum garnet (Nd:YAG) laser operated at various harmonics for photodetachment, and a magnetic bottle electron energy analyzer with a resolution of 35 meV at $EKE = 1$ eV. The photoelectron spectra were calibrated against the well-known photoelectron spectrum of Cu^- .² In this experiment, carbon aluminum hydride clusters were generated by a pulsed arc cluster ionization source (PACIS), which has been described in detail elsewhere.³ This PACIS source has been proven to be a powerful tool for generating metal and metal hydride cluster anions.⁴⁻¹⁴ In brief, a ~ 30 μs long, 150 V, 1000 A electrical pulse applied across the anode and sample cathode of the discharging chamber vaporizes the aluminum and carbon atoms and forms plasma. In this case the cathode was prepared by mixing and pressing aluminum and carbon powder into a well drilled hole on the top of an aluminum rod. About 200 psi of ultrahigh purity hydrogen gas was then injected into the arc region, and broken into H atoms. The plasma mix was then flushed down in a 20 cm flow tube, where it reacted, formed clusters and cooled. Anions generated by this method are at a temperature of 450 K.⁴ The anions were then mass-selected for photoelectron spectroscopic studies. The high power of this PACIS source and its ability of breaking molecules and metals into atoms turn out to be the key of generating metal hydride clusters in the gas phase, while other conventional ion sources, such as laser vaporization source, cannot make these novel clusters.

The global, unbiased, isomeric search for CA_4H and CA_4H^- were done by using the home-developed “grid” program.¹⁵⁻²¹ In this strategy, a three-dimensional box containing 6x6x6 grid points are built up. The distance between the neighboring grid points is set to the averaged value of H-H, C-H, C-Al and Al-Al single bonds. The five heavy atoms (one C and four Al) and one H-atom are placed onto these grid sites to exhaustively sort possible effective sets. If no atoms or groups are completely separated from the remaining parts, the structure can be considered as an effective starting structure for the CA_4H or CA_4H^- . In each system, we have totally 2026 input structures. The geometry and frequency calculations of the initial structures were computed at the B3LYP²²⁻²⁴/6-31G(d)²⁵ level. We totally obtained 32 local minima for CA_4H^- and 41 local minima for CA_4H , all of which have all positive frequency values. Then, we performed CBS-QB3 calculations²⁶ for all the minima. In order to improve the accuracy, high level B3LYP/aug-cc-pVTZ²⁷ (for geometry and vibrational frequencies) and

CCSD(T)^{28,29} /aug-cc-pVTZ (for single-point energy) calculations are performed for all the low-lying isomers ($\Delta E < 10$ kcal/mol at CBSQB3 level). Natural bond orbital (NBO)^{30,31} analyses at the B3LYP/aug-cc-pVTZ level were also carried out. All calculations were performed using the Gaussian 03³² and Gaussian 09³³ program packages.

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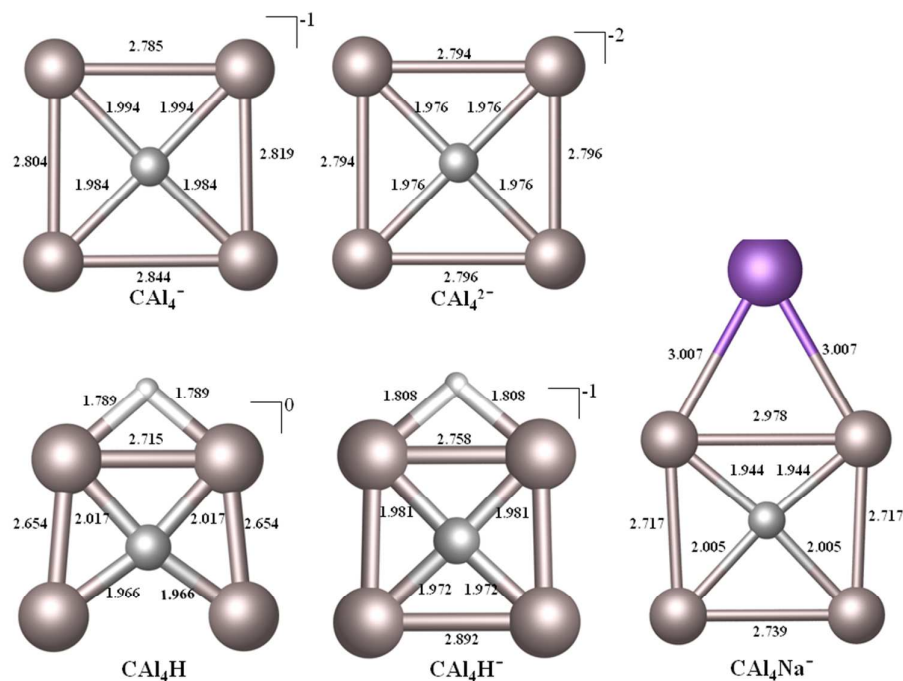


Figure S1. The key structural parameters of Al_4^- , Al_4^{2-} , Al_4H , Al_4H^- and Al_4Na^- at the level of B3LYP/aug-cc-pVTZ.

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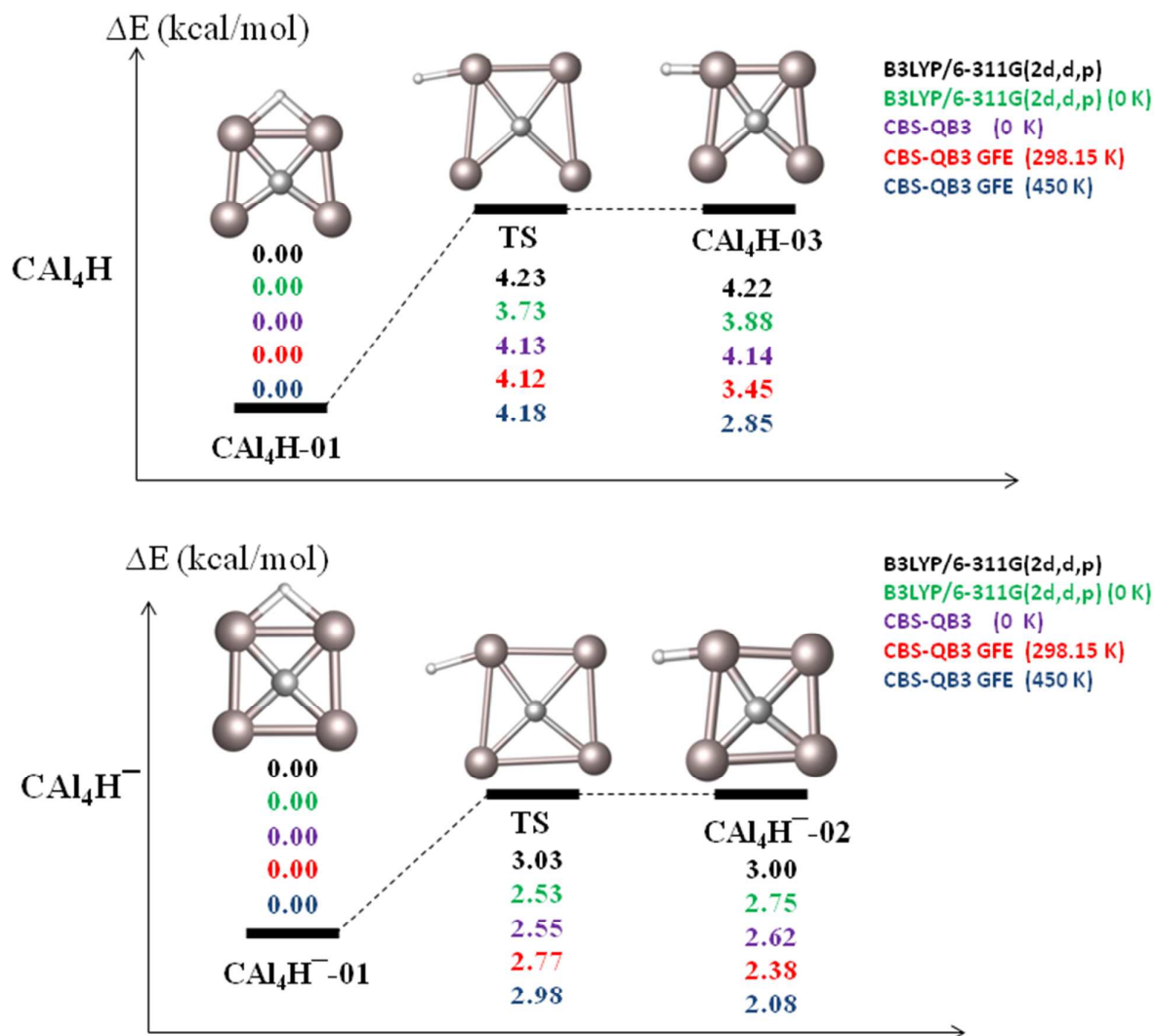


Figure S2. The conversion between CAI₄H-01 and CAI₄H-03, CAI₄H⁻-01 and CAI₄H⁻-02. The black values are the energy differences at the level of B3LYP/6-311G(2d,d,p), green values are corrected with zero-point energy, and purple values are at the level of CBS-QB3 with zero-point energy correction. Red and blue values are the Gibbs free energy differences at CBS-QB3 level at 298.15K and 450K.

4.

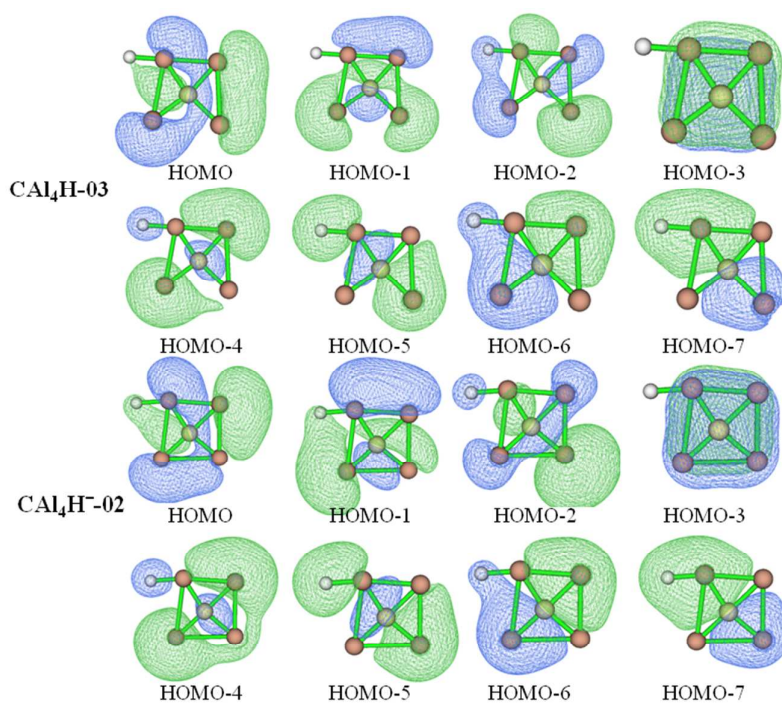
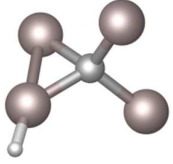
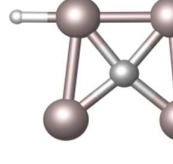
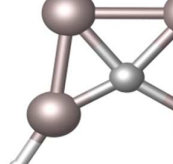
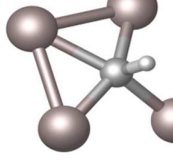


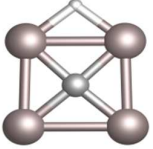
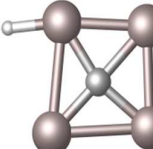
Figure S3. Molecular orbitals of neutral CA_4H-03 and anion $CA_4H^- -02$ with the terminal-H ptC at the level of B3LYP/aug-cc-pVTZ.

5. Structures, total energies (E), zero-point energies (ZPE) and the Cartesian coordinates all the low-lying CA_4H isomers ($\Delta E < 10\text{kcal/mol}$) at the levels of B3LYP/aug-cc-pVTZ and CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ. All the energies are in Hartree.

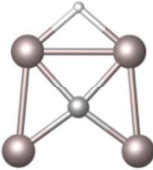
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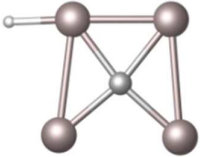
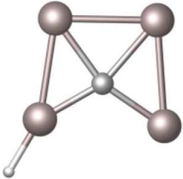
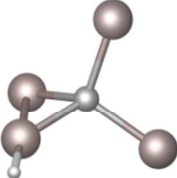
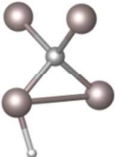
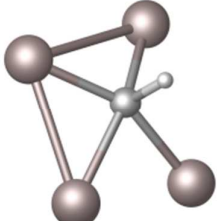
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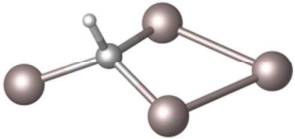
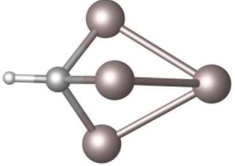
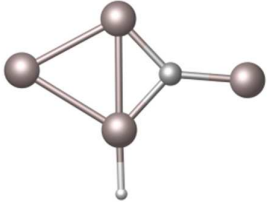
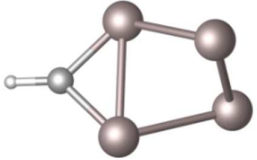
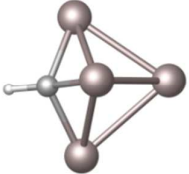
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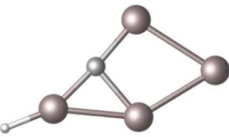


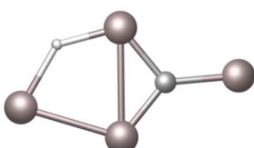
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	E= -1008.56782972 ZPE=0.013015 13 0 1.375725 -1.347696 0.000000 1 0 -0.006618 -2.513768 0.000000 6 0 0.000191 0.078375 0.000000 13 0 1.450012 1.415520 0.000000 13 0 -1.382821 -1.340446 0.000000 13 0 -1.442603 1.423085 0.000000	E= -1006.6743261 6 0 0.002068 0.154093 0.000000 13 0 1.951227 0.471255 0.000000 13 0 -0.551007 2.014855 0.000000 13 0 -1.720356 -0.715107 0.000000 13 0 0.556000 -1.857126 0.000000 1 0 -3.049486 0.206482 0.000000
	E=-1008.56309743 ZPE=0.012717 13 0 1.375725 -1.347696 0.000000 1 0 -0.006618 -2.513768 0.000000 6 0 0.000191 0.078375 0.000000 13 0 1.450012 1.415520 0.000000 13 0 -1.382821 -1.340446 0.000000 13 0 -1.442603 1.423085 0.000000	E=-1006.6698457 6 0 0.002068 0.154093 0.000000 13 0 1.951227 0.471255 0.000000 13 0 -0.551007 2.014855 0.000000 13 0 -1.720356 -0.715107 0.000000 13 0 0.556000 -1.857126 0.000000 1 0 -3.049486 0.206482 0.000000

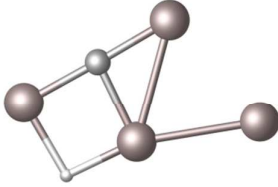
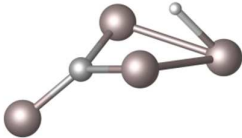
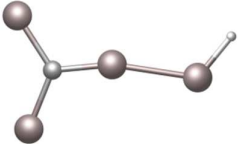
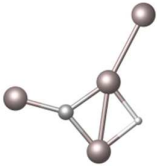
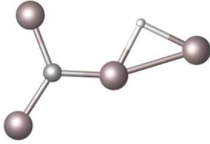
7. Structures, total energies and Cartesian coordinates of 41 isomers of CaI_4H at the level of CBS-QB3 with zero-point energy correction.

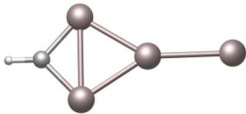
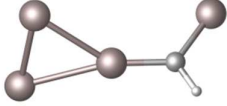

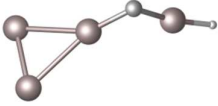
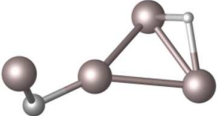
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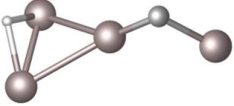
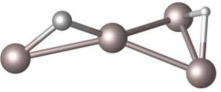
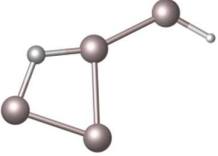
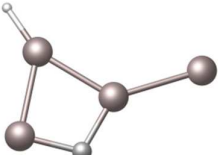
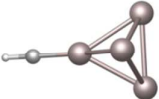
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	<p>E= -1006.579424</p> <p>1 -1.242067 -0.960904 2.681660</p> <p>13 -1.247118 -0.397181 1.199280</p> <p>13 -1.411646 0.419723 -1.315267</p> <p>13 1.357637 -1.526989 -0.428875</p> <p>13 1.322280 1.570974 0.364181</p> <p>6 0.161182 0.016009 -0.055466</p>
	<p>E= -1006.577905</p> <p>13 1.421409 0.016572 -1.414677</p> <p>1 2.558218 -0.014714 1.321824</p> <p>13 -1.269242 -1.615335 -0.117583</p> <p>6 -0.105581 0.000994 -0.072595</p> <p>13 -1.266181 1.619903 -0.082295</p> <p>13 0.965958 -0.020468 1.546381</p>
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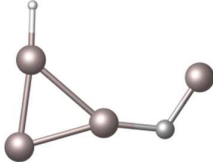
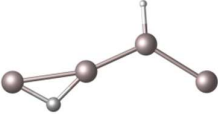
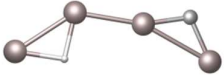
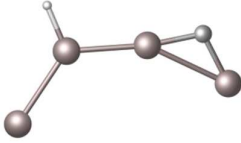
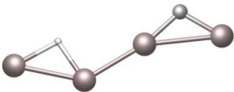
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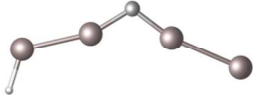
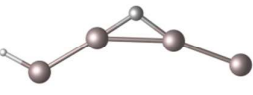
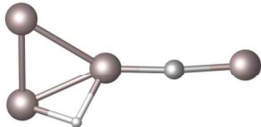
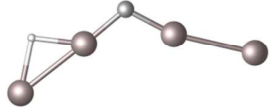
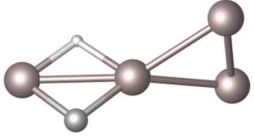
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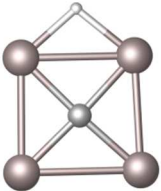
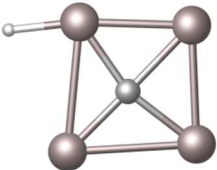
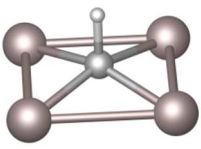
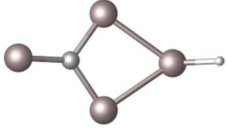
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	<p>E= -1006.505762</p> <p>1 -1.604789 -2.647864 -0.009761</p> <p>13 -1.238359 -1.109953 -0.005513</p> <p>13 1.381815 -0.193984 1.287893</p> <p>13 -0.448625 1.428057 0.006354</p> <p>6 -2.077828 0.564622 -0.001507</p> <p>13 1.387612 -0.181033 -1.287288</p>
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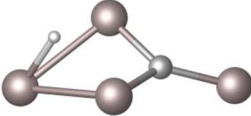
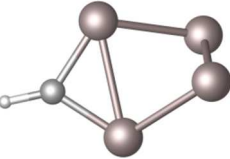
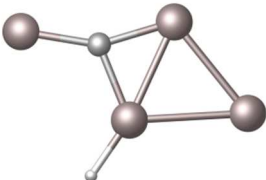
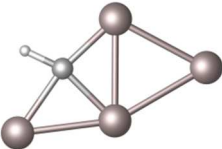
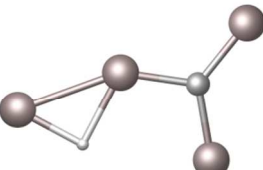
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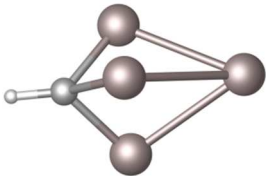
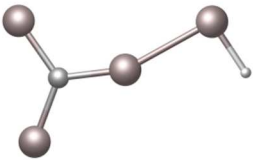
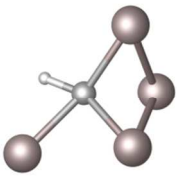
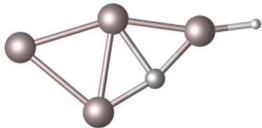
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	<p>E= -1006.475340</p> <p>13 3.869782 -0.759057 -0.000324</p> <p>13 1.635697 0.948292 0.000299</p> <p>1 1.691945 2.551473 0.000477</p> <p>13 -0.832875 0.114969 0.000296</p> <p>6 -2.248461 -1.049120 0.001471</p> <p>13 -3.765002 -0.016261 -0.000986</p>
	<p>E= -1006.472335</p> <p>13 -1.122582 -3.821191 0.000000</p> <p>13 -1.485441 -1.133348 0.000000</p> <p>1 -0.079444 -2.246895 0.000000</p> <p>13 0.000000 1.055395 0.000000</p> <p>6 0.532780 2.808527 0.000000</p> <p>13 2.368236 2.775739 0.000000</p>
	<p>E= -1006.471348</p> <p>13 2.790377 2.038003 0.000000</p> <p>6 1.051694 2.620844 0.000000</p> <p>13 0.000000 1.120219 0.000000</p> <p>1 -3.246136 -0.170449 0.000000</p> <p>13 -1.768076 -0.794913 0.000000</p> <p>13 -1.257995 -3.559818 0.000000</p>
	<p>E= -1006.471180</p> <p>13 0.779114 -4.014857 0.000000</p> <p>13 -0.596131 -1.675183 0.000000</p> <p>1 1.129432 -2.160788 0.000000</p> <p>13 0.000000 0.905076 0.000000</p> <p>13 -0.623926 3.765567 0.000000</p> <p>6 0.767139 2.568827 0.000000</p>

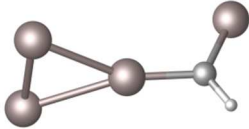
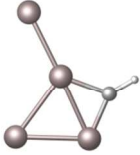
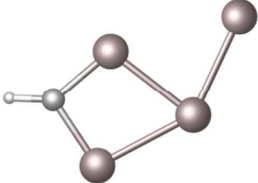
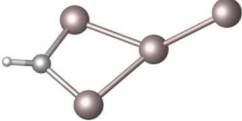
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	<p>E= -1006.469666</p> <p>13 4.096508 -0.681380 0.005250</p> <p>13 1.498423 0.329720 -0.005846</p> <p>6 0.056753 1.429322 -0.014248</p> <p>13 -1.480772 0.488238 0.011221</p> <p>13 -3.745224 -0.795862 -0.011894</p> <p>1 -5.136681 -0.005240 0.102000</p>
	<p>E= -1006.468433</p> <p>13 3.835949 0.122700 0.032710</p> <p>6 1.882029 -0.063687 0.015221</p> <p>13 -0.001518 -0.139645 -0.149396</p> <p>1 -0.804838 -1.252466 1.019555</p> <p>13 -2.259289 -1.250348 -0.011458</p> <p>13 -2.381859 1.393031 0.042693</p>
	<p>E= -1006.464911</p> <p>13 -3.838826 -0.941267 0.000000</p> <p>13 -1.528842 0.437071 0.000000</p> <p>1 -3.230228 0.864288 0.000000</p> <p>6 0.000000 1.420320 0.000000</p> <p>13 1.496869 0.377085 0.000000</p> <p>13 4.119279 -0.594905 0.000000</p>
	<p>E=-1006.465952</p> <p>13 -2.949431 0.020644 -0.406115</p> <p>6 -1.894379 -0.062522 1.127881</p> <p>1 -1.425209 0.065726 -1.308913</p> <p>13 -0.312746 -0.019084 0.133547</p> <p>13 2.107181 1.262266 -0.052979</p> <p>13 2.138957 -1.240026 -0.094328</p>

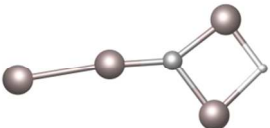
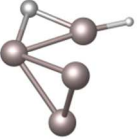
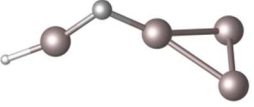
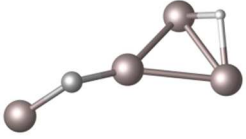
8. Structures, total energies and Cartesian coordinates of 32 isomers of CaI_4H^- at the level of CBS-QB3 with zero-point energy correction.

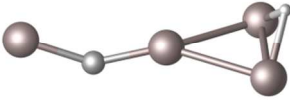
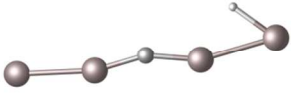
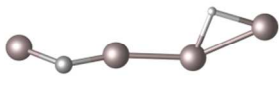
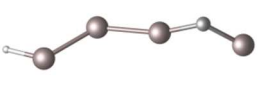
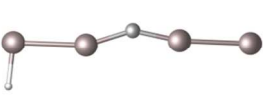
	<p>E= -1006.680631</p> <p>13 1.337472 -1.383936 -0.000066</p> <p>13 1.347142 1.375327 -0.000262</p> <p>6 -0.078640 0.000600 -0.000074</p> <p>13 -1.416057 1.450109 0.000263</p> <p>13 -1.424932 -1.441075 0.000084</p> <p>1 2.504713 -0.009125 0.000197</p>
	<p>E= -1006.676447</p> <p>1 0.849157 2.933799 0.001444</p> <p>13 -0.333207 1.832983 0.000413</p> <p>6 0.150412 -0.032606 -0.000555</p> <p>13 -1.934398 -0.147647 -0.000442</p> <p>13 0.046535 -2.005785 0.000556</p> <p>13 2.086329 0.109821 -0.000383</p>
	<p>E= -1006.660326</p> <p>1 -1.389650 -0.000782 0.000000</p> <p>6 -0.268074 -0.000124 0.000000</p> <p>13 0.057656 -1.436448 1.436652</p> <p>13 0.057656 1.436506 1.436279</p> <p>13 0.057656 -1.436448 -1.436652</p> <p>13 0.057656 1.436506 -1.436279</p>
	<p>E= -1006.647914</p> <p>1 3.531871 -0.005781 1.376546</p> <p>13 2.454510 -0.003082 0.131133</p> <p>13 0.238981 -1.514065 -0.210489</p> <p>13 0.244110 1.516787 -0.209221</p> <p>6 -0.919767 0.003424 -0.099592</p> <p>13 -2.784775 -0.000775 0.228655</p>

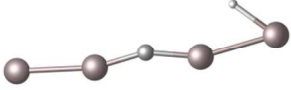
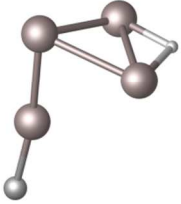
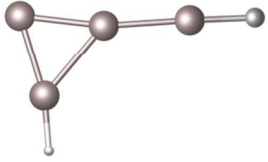
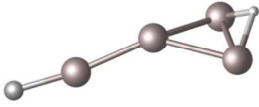
	<p>E= -1006.645228</p> <p>13 -2.420224 0.000083 0.584545</p> <p>13 -0.287478 1.467935 -0.426157</p> <p>13 -0.287605 -1.467876 -0.426177</p> <p>6 0.897193 0.000053 -0.127836</p> <p>13 2.710214 -0.000062 0.403409</p> <p>1 -1.676947 -0.001364 -0.996053</p>
	<p>E= -1006.641318</p> <p>6 -2.134281 -0.005904 -0.000371</p> <p>13 -0.793408 -1.146397 -0.679067</p> <p>13 -0.802347 1.144806 0.678886</p> <p>13 1.417483 -1.050525 0.738863</p> <p>13 1.411256 1.055619 -0.738411</p> <p>1 -3.223115 -0.010114 -0.001288</p>
	<p>E=-1006.640901</p> <p>1 -2.700762 -0.457785 0.000000</p> <p>13 -1.087925 -0.484355 0.000000</p> <p>13 -0.788247 2.837966 0.000000</p> <p>13 0.629466 -2.755131 0.000000</p> <p>13 1.454457 -0.079274 0.000000</p> <p>6 0.000000 1.118017 0.000000</p>
	<p>E= -1006.640088</p> <p>13 -2.713798 -0.303112 0.000020</p> <p>6 -0.952323 0.806552 -0.000027</p> <p>13 -0.193888 -1.009514 -0.000028</p> <p>13 0.861073 1.472813 -0.000006</p> <p>13 2.616308 -0.657541 0.000020</p> <p>1 -1.692108 1.626288 0.000085</p>
	<p>E= -1006.638967</p> <p>1 -1.986324 0.767541 0.000000</p> <p>13 -2.060351 2.539712 0.000000</p> <p>13 0.000000 0.904870 0.000000</p> <p>13 2.598607 -1.052630 0.000000</p>

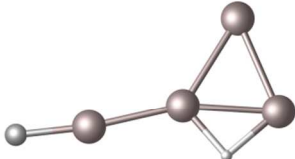
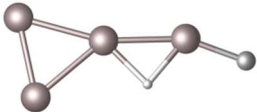
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	<p>E= -1006.635687</p> <p>6 0.500520 -0.976291 0.000000</p> <p>13 -0.886468 -2.277307 0.000000</p> <p>13 2.354101 -1.389864 0.000000</p> <p>13 0.000000 0.816366 0.000000</p> <p>13 -1.665845 2.986422 0.000000</p> <p>1 -0.426369 4.094721 0.000000</p>
	<p>E= -1006.634628</p> <p>13 1.404520 -1.346530 -0.227028</p> <p>13 1.403978 1.347347 -0.224390</p> <p>13 -0.473414 -0.001839 1.418206</p> <p>6 -0.155127 0.000758 -0.641689</p> <p>1 -0.445970 0.001928 -1.717457</p> <p>13 -2.229181 0.000524 -0.538512</p>
	<p>E= -1006.631816</p> <p>1 4.034234 0.627523 0.000000</p> <p>13 2.435232 0.521978 0.000000</p> <p>13 0.000000 1.014991 0.000000</p> <p>6 1.083065 -0.748885 0.000000</p> <p>13 -0.574813 -1.604876 0.000000</p> <p>13 -2.670621 0.365275 0.000000</p>

	<p>E= -1006.618685</p> <p>13 3.146686 0.000190 -0.611058</p> <p>6 1.924160 -0.000330 0.828722</p> <p>1 2.198845 -0.000638 1.890913</p> <p>13 0.093693 -0.000178 0.466270</p> <p>13 -2.148889 -1.219257 -0.191764</p> <p>13 -2.148705 1.219446 -0.191391</p>
	<p>E= -1006.603111</p> <p>1 2.673965 1.239249 0.000000</p> <p>6 1.916831 0.455918 0.000000</p> <p>13 1.678399 -1.403014 0.000000</p> <p>13 0.000000 0.605742 0.000000</p> <p>13 -1.787491 2.569839 0.000000</p> <p>13 -0.981289 -2.078318 0.000000</p>
	<p>E= -1006.602450</p> <p>13 2.891339 -0.278592 0.000000</p> <p>13 0.375270 -1.270996 0.000000</p> <p>13 0.000000 1.285828 0.000000</p> <p>6 -1.863013 1.389389 0.000000</p> <p>1 -2.624854 2.168985 0.000000</p> <p>13 -2.204845 -0.544341 0.000000</p>
	<p>E= -1006.600493</p> <p>1 -3.264879 0.004026 1.239849</p> <p>6 -2.431709 0.002563 0.533742</p> <p>13 -1.364971 -1.460101 -0.065628</p> <p>13 -1.360593 1.461092 -0.067395</p> <p>13 0.761624 -0.002768 -0.553474</p> <p>13 3.337412 0.000285 0.344781</p>

	<p>E= -1006.593055</p> <p>1 1.052188 3.156103 0.000000</p> <p>13 -0.626257 2.608956 0.000000</p> <p>6 0.000000 0.771484 0.000000</p> <p>13 1.896053 1.397764 0.000000</p> <p>13 -0.464814 -0.981029 0.000000</p> <p>13 -0.885919 -3.624537 0.000000</p>
	<p>E= -1006.583795</p> <p>1 -1.500282 2.645771 -0.001676</p> <p>13 -1.214963 1.072768 -0.000777</p> <p>13 1.409160 0.150678 -1.318732</p> <p>13 -0.475338 -1.324173 -0.000447</p> <p>6 -2.187407 -0.549573 -0.000457</p> <p>13 1.406119 0.150854 1.320296</p>
	<p>E= -1006.572962</p> <p>6 -1.899007 -0.000702 1.009978</p> <p>13 -2.989595 0.000214 -0.411227</p> <p>1 -4.287753 0.000912 -1.347225</p> <p>13 -0.153785 -0.000273 0.384129</p> <p>13 2.174672 1.210770 -0.167431</p> <p>13 2.175000 -1.210457 -0.167982</p>
	<p>E= -1006.572515</p> <p>1 2.654677 0.042699 0.942856</p> <p>13 2.226225 -1.218595 -0.248504</p> <p>13 2.037730 1.377567 -0.074178</p> <p>13 -0.227988 -0.140815 0.275517</p> <p>6 -1.959664 -0.325285 0.771620</p> <p>13 -3.335713 0.128690 -0.381495</p>

	<p>E= -1006.569560</p> <p>1 2.676902 0.000199 1.094061</p> <p>13 2.236798 1.326670 -0.009461</p> <p>13 2.237162 -1.326476 -0.009376</p> <p>13 -0.144077 -0.000131 -0.009669</p> <p>6 -1.891598 -0.000367 -0.475108</p> <p>13 -3.662754 0.000091 0.163628</p>
	<p>E= -1006.566719</p> <p>1 0.555639 -3.027417 0.000000</p> <p>13 1.924102 -1.873485 0.000000</p> <p>13 -1.131211 -2.427893 0.000000</p> <p>13 0.000000 0.034371 0.000000</p> <p>6 -0.323285 1.808843 0.000000</p> <p>13 -0.686424 3.665035 0.000000</p>
	<p>E= -1006.551277</p> <p>13 4.142841 0.353573 0.093650</p> <p>13 1.691960 -0.444246 -0.314332</p> <p>1 2.456415 0.971239 0.520926</p> <p>13 -0.828013 -0.177807 0.108796</p> <p>6 -2.545475 -0.388816 0.623040</p> <p>13 -4.020909 0.373222 -0.215743</p>
	<p>E= -1006.543564</p> <p>1 -5.298560 -0.003323 -0.168367</p> <p>13 -3.812674 -0.665668 0.015955</p> <p>13 -1.692283 0.816241 -0.171943</p> <p>13 0.762290 0.154836 0.151024</p> <p>6 2.483997 0.077390 0.692318</p> <p>13 4.003788 -0.340871 -0.301616</p>
	<p>E= -1006.541796</p> <p>13 -4.299708 -0.910762 0.000000</p> <p>13 -1.604809 -0.439733 0.000000</p> <p>1 -4.134188 -2.565675 0.000000</p> <p>6 0.000000 0.465835 0.000000</p>

	<p>13 1.799425 0.446637 0.000000</p> <p>13 4.423107 0.886216 0.000000</p>
	<p>E= -1006.541235</p> <p>13 4.036571 -1.626467 0.000000</p> <p>13 1.498414 -0.939062 0.000000</p> <p>1 3.356494 -0.005077 0.000000</p> <p>6 0.000000 0.149369 0.000000</p> <p>13 -1.737650 0.609816 0.000000</p> <p>13 -4.055527 1.887164 0.000000</p>
	<p>E= -1006.464416</p> <p>6 -3.359753 0.602825 0.000000</p> <p>13 -1.450567 0.717058 0.000000</p> <p>13 0.968542 1.229008 0.000000</p> <p>13 0.968542 -1.033326 1.440240</p> <p>13 0.968542 -1.033326 -1.440240</p> <p>1 1.242756 -2.049330 0.000000</p>
	<p>E= -1006.462954</p> <p>6 4.427296 0.072418 0.000000</p> <p>13 2.523243 0.240308 0.000000</p> <p>13 0.000000 0.399467 0.000000</p> <p>13 -2.420140 1.002645 0.000000</p> <p>13 -1.988352 -1.440484 0.000000</p> <p>1 -2.055539 -3.059663 0.000000</p>
	<p>E= -1006.456835</p> <p>6 -4.364845 0.000526 -0.184625</p> <p>13 -2.465504 -0.000340 -0.080857</p> <p>13 -0.035919 0.000001 0.441876</p> <p>13 2.141852 1.368573 -0.158013</p> <p>1 3.019559 0.000010 0.523137</p> <p>13 2.141841 -1.368478 -0.158036</p>

	<p>E= -1006.455153</p> <p>6 -4.356054 0.285086 -0.000094</p> <p>13 -2.483542 -0.079931 0.000010</p> <p>1 0.681179 -1.889701 0.000070</p> <p>13 0.010323 -0.270632 0.000030</p> <p>13 2.338043 -1.169276 0.000006</p> <p>13 2.093264 1.533623 -0.000008</p>
	<p>E= -1006.449874</p> <p>6 4.253248 -0.190871 0.000000</p> <p>13 2.445874 0.424187 0.000000</p> <p>13 0.000000 0.297042 0.000000</p> <p>1 1.338686 -0.980910 0.000000</p> <p>13 -2.544953 0.916467 0.000000</p> <p>13 -1.966935 -1.474147 0.000000</p>