Supporting Information

A DFT study of endocyclic allenes - unprecedentedly superbasic hydrocarbons

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1. Computational details

Computational Details

All geometrical optimizations were carried out employing B3LYP hybrid functional DFT method (Becke's 3 parameter functional with the non-local correlation provided by the expression of Lee et al.)\(^1\) as well as M052X\(^2\) and M062X\(^3\) hybrid functionals of Truhlar and Zhao employing 6-31G* basis set. Calculations were performed using Gaussian03 suite of programs,\(^4\) implemented on dual core Opteron 240 personal computer under Linux operating system and computer cluster Isabella at the Computing center of the University of Zagreb (Isabella computer cluster (24 dual processor HP ProLiant BLP20p nodes with Intel Xeon 2.8 GHz, 32 dual processor Dell 1850 1U nodes with Intel Xeon 3.4 GHz and 24 dual processor Pyramid GX28 nodes with AMD Opteron 248). Harmonic vibration frequencies were calculated for all localized stationary structures to verify minima by no possession of imaginary vibrations. Single point calculations were conducted using B3LYP/6-311+G**//B3LYP/6-31G* method, and the gas phase basicity (GB) were calculated as the Gibbs free energy change of the protonation reaction. Throughout the manuscript, B3LYP\(^5\) denotes PA calculated at B3LYP/6-31G*+E\(_{\text{vib}}\)(B3LYP/6-31G*), while B3LYP(2)\(^6\) denotes the PA obtained at the B3LYP/6-311+G**//B3LYP/6-31G**+E\(_{\text{vib}}\)(B3LYP/6-31G*) level. Likewise, notation for M052X, M052X(2), M062X and M062X(2) was applied. Hybridization, Wiberg and BOAO bond orders were obtained from NBO analysis incorporated within Gaussian03 program using pop=nboread keyword.

Proton affinity of allenes in the gas phase (PA\(_{\text{B3LYP}(2)}\)) was calculated using the following equations:\(^6\)

\[
\text{PA}(B) = \Delta E_{\text{el}} + \Delta \text{ZPVE}_{\text{B3LYP}}
\]

\[
\Delta E_{\text{el}} = E(B)_{\text{B3LYP}(2)} - E(BH^+)_{\text{B3LYP}(2)}
\]

\[
\Delta \text{ZPVE}_{\text{B3LYP}} = \text{ZPVE}(B)_{\text{B3LYP}} - \text{ZPVE}(BH^+)_{\text{B3LYP}}
\]
Here B3LYP denotes B3LYP/6-31G* level; while B3LYP(2) is B3LYP/6-311+G**//B3LYP/6-31G* model. Similarly, PA\textsubscript{M052X(2)} and PA\textsubscript{M062X(2)} were obtained.

Gas phase basicities (GB) of allenes are defined as a negative value of the free energy change for the protonation reaction.

The solvent effect in acetonitrile was estimated by employing the polarized continuum model at IPCM/B3LYP/6-311+G** //B3LYP//6-31G* level\textsuperscript{7}. The molecular surface determining a cavity within a solvent is obtained by the isodensity shell of 0.0004eB\textsuperscript{-3}, thus giving rise to the isodensity polarized continuum model (IPCM)\textsuperscript{8} utilizing dielectric constant for acetonitrile $\varepsilon = 36.64$. Estimation of PA and pK\textsubscript{a} values in acetonitrile was achieved by using the equations derived for guanidines\textsuperscript{9}.

\begin{align*}
pK_a &= 0.4953PA(B\text{MeCN}) - 119.7 \text{ units} \quad (4) \\
PA(B\text{MeCN}) &= \Delta E_{el \text{ MeCN}} + \Delta ZPVE\text{B3LYP} \quad (5) \\
\Delta E_{el \text{ MeCN}} &= E(B\text{MeCN}) - E(BH^+\text{MeCN}) \quad (6) \\
\Delta ZPVE\text{B3LYP} &= ZPVE(B\text{B3LYP}) - ZPVE(BH^+\text{B3LYP}) \quad (7)
\end{align*}

In these equations MeCN denotes IPCM/B3LYP/6-311+G**//B3LYP/6-31G* model and B3LYP denotes B3LYP/6-31G* method, hence PA\textsubscript{MeCN} = IPCM/6-311+G**//B3LYP/6-31G* + $E_{vib}(B3LYP/6-31G^*)$\textsuperscript{10}. 
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\(^a\) 1.80 denotes \( sp^{1.80} \)
Table SI-2. Gas phase proton affinities, basicities (kcal mol\(^{-1}\)) and pKa values.

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\(^a\) \(\text{PA}_{\text{B3LYP}}\): B3LYP/6-31G*\(^+\)\(E_{\text{vib}}\)(B3LYP/6-31G*)\(^a\); \(^b\) \(\text{PA}_{\text{B3LYP}(2)}\): B3LYP/6-311+G**/B3LYP/6-31G*\(^+\)\(E_{\text{vib}}\)(B3LYP/6-31G*)\(^b\); \(^c\) B3LYP/6-31G*; \(^d\) \(\text{PA}_{\text{M05X}(2)}\): M05X/6-311+G**/M05X/6-31G*\(^+\)\(E_{\text{vib}}\)(M05X/6-31G*); \(^e\) \(\text{PA}_{\text{M06X}}\): M06X/6-311+G**/M06X/6-31G*\(^+\)\(E_{\text{vib}}\)(M06X/6-31G*)
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| H | 4.68436200 | -1.17428200 | 0.21437000 |
| C | 3.05204700 | 0.12792200 | -0.36013400 |
| C | -3.02807400 | 0.02417700 | 0.37797800 |
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Allene 17 B3LYP/6-31G*

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Allene 10H B3LYP/6-31G*

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C                  2.532556    0.000133   -1.220123  
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Allene 12H B3LYP/6-31G*

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C                  -0.69769300    1.17391000   -0.00005700  
C                   1.21928700   -1.35468100   -0.00000200  
C                   0.71748500    1.13421800    0.00002400  
C                   1.57552600    0.02615600    0.00006100  
C                  -2.58099900   -2.07790000    0.00021200  
H                  -2.65620700   -2.73746000    0.87801000  
C                  -3.62912200   -1.01225200   -0.00016400  
H                 -4.69323400   -1.21721500   -0.00040700  
C                 -3.05552500    0.21029800   -0.00012900  
C                  3.03357700    0.11180100    0.00014300  
C                   2.49514100   -2.16764600   -0.00011100  
H                  -2.55573200   -2.82867000    0.87746800  
C                   3.57029300   -1.12652400   -0.00019400  
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H                   -3.58494800    1.15443700   -0.00022200  
H                    3.58769100    2.54774000   -0.00004000  
C                  -1.11360600    2.57374000   -0.00004000  
H                  -2.14411900    2.90463900   -0.00015500  
C                   -0.02947900    3.37680800    0.00002500  
H                   -0.03713400    4.46036100   -0.00010100  
C                   1.22294500    2.55971800    0.00011300  
H                   1.85209000    2.76896600    0.87818700  
H                   1.85237500    2.76901600   -0.87773300  
H                   -0.06503700   -3.02345300    0.00005300 

Allene 13H B3LYP/6-31G*

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C                   -0.70168100    2.54773100   -0.12905000  
C                  -1.56388300    1.49726700   -0.20046500  
C                  -1.29239800    0.08509500   -0.03391100  
C                   0.70171400    2.54772100    0.12906900  
C                   -0.00000200   -0.48559200   -0.00001700  
C                   1.56390400    1.49724500    0.20046000  
C                   1.29239800    0.08508300    0.03388100  
H                   -1.14490300    3.53107000   -0.26434200  
H                   -2.59336700    1.76340500   -0.39969000
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**Allene 15H B3LYP/6-31G***

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Allene 16H B3LYP/6-31G*

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Allene 17H B3LYP/6-31G*

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H  6.68570200  4.80913900  0.00005900  
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Allene 18H B3LYP/6-31G*  

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C  -0.73351200  -2.07698400  -0.02567400  
C   1.26194300   0.40608100  -0.02554700  
C   0.72522500  -2.11249900  -0.02956700  
C   1.60046300  -1.03239100  -0.02100100  
C  -2.46388800   1.16695500  -0.01877200  
H   -2.49799300   2.25088100  -0.02039300  
C   -3.55132400  -0.28199000  -0.01555800  
C   -3.04235300  -1.06559900  -0.01661300  
C    3.04252700  -1.08399000  -0.01014500  
C    2.48055900   1.15147400  -0.02488400  
H    2.50872700   2.23522500  -0.02748200  
C     3.55432000   0.27176900  -0.01590900  
C     1.12291900  -3.49714000  -0.05115600  
H     2.15116700  -3.82158600  -0.08570800  
C     0.03090800  -4.32965800  -0.04223500  
C    -1.23658500  -3.50782800  -0.03562000  
H    -1.85995800  -3.72227200   0.84406400  
H    -1.86297000  -3.70353800  -0.91720200  
C    -4.10872900  -1.95621400  -0.01408600  
H    -4.07932100  -3.03683000  -0.01341000  
C     4.12485300  -1.96299500   0.01091400  
H     4.11029800  -3.04547500   0.02827800  
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C     4.99543700   0.22530300  -0.00300600  
C    -4.98361000   0.23206300  -0.01192100  
C    -5.32146900  -1.20126000  -0.01083300  
C     5.87071100  -1.29875700  -0.00875500  
C     6.61405800  -1.77616600   0.03708800  
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C    -6.59810600  -1.77550700  -0.00506000  
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C     7.84385220  -1.14904500   0.04031100  
C    -7.28914600  -1.33653200  -0.00267600  
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H   5.48363700  6.66502900  0.08277300
H   5.35444400  5.80612400 -1.46968600
H   4.54712100  5.17036000  -0.01666400
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C  12.02710800 -2.51299700  0.36378500
H  11.33327400 -3.27449800  0.00301200
H  12.99163600 -2.67961200  1.44822400
H  12.16105300 -2.64802100 -0.12416400
C  12.50190600 -0.08982700  0.09474000
H  13.49875400 -0.47223000 -0.13590400
H  12.24835800  0.67530800  0.64553900
H  12.52639600  0.38004700  1.08937500

Allene 19H B3LYP/6-31G*

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C   1.59235700  0.95558600  -0.08535200
C   1.24923100 -0.49063500  -0.06805000
C  -0.00992800 -1.08230800  -0.00704100
C    0.72015900  2.03303300  -0.04466600
C   2.45546500  2.05230900   0.02495200
C   3.53908100  0.34963000  -0.17693700
C   3.01723700  1.00499900  -0.15299400
C  -3.02714500  1.02711900   0.13966700
C  -2.46758100  1.21450300   0.11261800
C  -2.49914400 -2.29779500   0.11202100
C  -3.54955200 -0.32912000   0.16464400
C  -1.12386700  3.45885600   0.04265700
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C  -0.07831500  5.35788100  -0.01133200
C   1.20995000  3.46969300  -0.07005700
C   1.87765700  3.68573100  -0.77177700
C   1.79286900  3.68351000  -0.97821300
C   4.10124600  1.89065900  -0.20857800
C   4.07484800  2.97297600  -0.21849500
C  -4.12225800  1.90912500   0.19855100
C  -4.10831700  2.99134300   0.21117200
C  -5.30874700  1.15333400   0.24420400
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### Allene 1 M052X/6-31G*

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### M052X

**Neutral**

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| C  | -1.22039800 | -1.03613600 | 0.35980000 |
| H  | 1.06229000 | 2.24823500 | 0.53618400 |
| H  | 2.61892100 | 0.45786400 | 0.51087800 |
| H  | 1.84258900 | -1.57590100 | -1.06363100 |
| H  | -1.06251100 | 2.24811400 | -0.53623400 |
| H  | -2.61895900 | 0.45756400 | -0.51101700 |
| H  | -1.84224100 | -1.57596100 | 1.06390600 |

### Allene 2 M052X/6-31G*

| C  | 0.36457900 | -0.61066000 | -0.10409600 |
| C  | 0.54038500 | 0.75632800 | -0.11387400 |
| C  | -0.56871700 | 1.64729500 | -0.42917800 |
| C  | -0.82816300 | -1.39029100 | -0.33625300 |
| C  | -1.70600600 | 1.23015600 | 0.10159200 |
| C  | -2.12362600 | -1.04807300 | -0.09002100 |
| C  | -2.44274000 | 0.22658500 | 0.54721700 |
| H  | -0.47403900 | 2.47050600 | -1.12782400 |
| H  | -0.65111100 | -2.39793500 | -0.70293200 |
| H  | -2.90449000 | -1.77068100 | -0.30638600 |
| H  | -3.14085800 | 0.29575000 | 1.37374600 |
| C  | 1.95741600 | 1.06548000 | 0.10436100 |
| H  | 2.35730700 | 2.06894600 | 0.14744500 |
| C  | 2.64943100 | -0.07907300 | 0.22666300 |
| H  | 3.71308700 | -0.17278300 | 0.39293100 |
| C  | 1.71912300 | -1.25060400 | 0.99469900 |
| H  | 1.74520900 | -1.89541000 | 0.97976200 |
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H   -0.56788400 -2.00566100 -1.00976900
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Allene 4 M052X/6-31G*

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C   0.52767500  1.47431900  0.08191500
C   2.00221100 -1.17054500  0.45363000
C   1.85906300  1.12451600 -0.38148800
C   2.54574400 -0.04717800 -0.30578700
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Allene 10 M052X/6-31G*

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**PROTONATED**

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Allene 19H M052X/6-31G*

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M062X

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Allene 8 M062X/6-31G*

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Allene 16 M062X/6-31G*

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Allene 7H M062X/6-31G*

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