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G1747-1

REVISION ARTICLE

Lithium and Cesium Ion-Pair Acidities of Some Terminal
Acetylenes and Aggregation in Tetrahydrofuran

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Supplementary material. Z-matrices for Gaussian program used for *ab initio* calculations. All structure optimizations, energy and frequency calculations were done at Hartree-Fock level of theory using 6-31+G* basis set. Parameters given are optimized ones.

HCCLi

0, 1

H

C 1, CH

X 2, 1. 1, 90.

C 2, CC 3, 90. 1, 180. 0

X 4, 1. 2, 90. 3, 0. 0

Li 4, CLi 5, 90. 2, 180. 0

CH = 1.0591

CC = 1.2137

CLi = 1.9237

HCCLi(H₂O)

0, 1

H

C 1, CH

X 2, 1. 1, 90.

C 2, CC 3, 90. 1, 180. 0

671747-2

X	4, 1.	2, 90.	3, 0.	0
Li	4, CLi	5, 90.	2, 180.	0
X	6, 1.	4, 90.	5, 0.	0
O	6, OLi	7, 90.	4, 180.	0
X	8, 1.	6, 90.	7, 0.	0
X	8, 1.	9, 90.	6, 180.	0
H	8, OH,	10, HOX	9, 90.	0
H	8, OH	10, HOX	9, -90.	0

CH = 1.0592

CC = 1.2151

CLi = 1.9444

OLi = 1.9282

OH = 0.9501

HOX = 53.6724

HCCLi(H₂O)₂

0, 1

H

C 1, CH

X 2, 1. 1, 90.

C 2, CC 3, 90. 1, 180. 0

X 4, 1. 2, 90. 3, 0. 0

Li 4, CLi 5, 90. 2, 180. 0

X 6, 1. 4, 90. 5, 0. 0

X 6, 1. 7, 90. 4, 180. 0

O 6, OLi 8, OLiX 7, 0. 0

O 6, OLi 8, OLiX 7, 180. 0

H 9, OH 6, HOLi 7, 90. 0

H 9, OH 6, HOLi 7, -90. 0

H 10, OH 6, HOLi 7, 90. 0

H 10, OH 6, HOLi 7, -90. 0

CH = 1.0593

CC = 1.217

CLi = 1.9842

G1747-3

OLi = 2.0131
 OH = 0.9486
 OLiX = 53.7174
 HOLi = 126.3352

$\text{HCCLi}(\text{H}_2\text{O})_3$

0, 1

H

C 1, CH

X 2, 1. 1, 90.

C 2, CC 3, 90. 1, 180. 0

X 4, 1. 2, 90. 3, 0. 0

Li 4, CLi 5, 90. 2, 180. 0

X 6, 1. 4, 90. 5, 0. 0

X 6, 1. 7, 90. 4, 180. 0

O 6, OLi 8, OLiX 7, 0. 0

O 6, OLi 8, OLiX 7, 120. 0

O 6, OLi 8, OLiX 7, 240. 0

H 9, OH 6, HOLi 8, 90. 0

H 9, OH 6, HOLi 8, -90. 0

H 10, OH 6, HOLi 8, 90. 0

H 10, OH 6, HOLi 8, -90. 0

H 11, OH 6, HOLi 8, 90. 0

H 11, OH 6, HOLi 8, -90. 0

CH = 1.0594

CC = 1.2189

CLi = 2.028

OLi = 2.0826

OH = 0.9479

OLiX = 62.9604

HOLi = 126.4926

$(\text{HCCLi})_2$

671747-4

0, 1				
X				
X	1, 1.			
Li	2, LiX	1, 90.		
Li	2, LiX	1, 90.	3, 180.	0
C	2, CX	1, 90.	3, dCLi	0
C	2, CX	1, 90.	5, 180.	0
C	2, CCX	1, 90.	3, dCCLi	0
C	2, CCX	1, 90.	7, 180.	0
X	7, 1.	2, 90.	1, 0.	0
X	8, 1.	2, 90.	1, 0.	0
H	7, HC	9, 90.	5, dHC	0
H	8, HC	10, 90.	6, dHC	0

LiX	=	1.2852
CX	=	1.6506
CCX	=	2.589
HC	=	1.0607
dCLi	=	87.678
dCCLi	=	109.3113
dHC	=	174.8851

(HCCLi)₂(H₂O)₂

0, 1				
X				
X	1, 1.			
Li	2, LiX	1, 90.		
Li	2, LiX	1, 90.	3, 180.	0
C	2, CX	1, 90.	3, dCLi	0
C	2, CX	1, 90.	5, 180.	0
C	2, CCX	1, 90.	3, dCCLi	0
C	2, CCX	1, 90.	7, 180.	0
X	7, 1.	2, 90.	1, 0.	0
X	8, 1.	2, 90.	1, 0.	0
H	7, HC	9, 90.	5, dHC	0

G1747-5

H	8, HC	10, 90.	6, dHC	0
O	2, OLi	1, 90.	3, dOLi	0
O	2, OLi	1, 90.	13, 180.	0
X	13, 1.	2, 90.	1, 0.	0
X	14, 1.	2, 90.	1, 0.	0
H	13, HO1	15, 90.	3, dHLi1	0
H	13, HO2	15, 90.	3, dHLi2	0
H	14, HO1	16, 90.	4, dHLi1	0
H	14, HO2	16, 90.	4, dHLi2	0

LiX = 1.3113

CX = 1.6819

CCX = 2.6653

HC = 1.0603

HO1 = 0.9475

HO2 = 0.9505

OLi = 3.2042

dCLi = 88.2765

dCCLi = 107.8146

dHC = 176.5524

dHLi1 = 141.6214

dHLi2 = -109.7718

dOLi = 12.3378

(HCCLi)₂(H₂O)₄

0, 1

X

X 1, 1.

Li 2, LiX 1, 90.

Li 2, LiX 1, 90. 3, 180. 0

C 2, CX 1, 90. 3, dCLi 0

C 2, CX 1, 90. 5, 180. 0

C 2, CCX 1, 90. 3, dCCLi 0

011747-6

C	2, CCX	1, 90.	7, 180.	0
X	7, 1.	2, 90.	1, 0.	0
X	8, 1.	2, 90.	1, 0.	0
H	7, HC	9, 90.	5, dHC	0
H	8, HC	10, 90.	6, dHC	0
X	2, 2.5	1, 90.	3, dXLi	0
X	2, 2.5	1, 90.	13, 180.	0
O	3, OLi	13, OLiX	2, 90.	0
O	3, OLi	13, OLiX	2, -90.	0
O	4, OLi	14, OLiX	2, 90.	0
O	4, OLi	14, OLiX	2, -90.	0
H	15, HO	3, HOLi	13, 90.	0
H	15, HO	3, HOLi	13, -90.	0
H	16, HO	3, HOLi	13, 90.	0
H	16, HO	3, HOLi	13, -90.	0
H	17, HO	4, HOLi	14, 90.	0
H	17, HO	4, HOLi	14, -90.	0
H	18, HO	4, HOLi	14, 90.	0
H	18, HO	4, HOLi	14, -90.	0

LiX = 1.2142

CX = 1.8238

CCX = 3.0415

HC = 1.0599

HO = 0.9478

OLi = 1.9939

OLiX = 56.0946

HOLi = 125.5867

dCLi = 90.0564

dCCLi = 90.1763

dHC = 179.9923

dXLi = 0.2673