Electronic Supplementary Information

Influence of stepwise oxidation on the structure, stability, and properties of planar pentacoordinate carbon species CAl_5^+

Rui Sun[a,b], Xue-Feng Zhao[a,b], Bo Jin[a,b], Bin Huo[a,b], Jian-Hong Bian[a,b], Xiao-Ling Guan[a,b], Caixia Yuan[a,b,*] and Yan-Bo Wu[a,b,*]

a The Key Lab of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan, 030006, People's Republic of China.

b The Key Lab of Chemical Biology and Molecular Engineering of Ministry of Education, Institute of Molecular Science, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China.

*To whom correspondence should be addressed.

E-mail: cxyuan@sxu.edu.cn (C.X.Y.) or wyb@sxu.edu.cn (Y.B.W.)

Contents

Cartesian coordinates of structures shown in Fig. 1.

B3LYP/aug-cc-pVTZ-optimized structures

0

C	0.00000000	0.00000000	0.00000000
Al	0.00000000	2.10535000	0.00000000
Al	2.00230700	0.65058900	0.00000000
Al	-1.23749400	-1.70326400	0.00000000
Al	-2.00230700	0.65058900	0.00000000
Al	1.23749400	-1.70326400	0.00000000

1a

C	0.00000000	0.00000000	0.22732200
Al	0.00000000	1.25682800	-1.45993900
Al	0.00000000	1.87229500	0.88145000
Al	0.00000000	0.00000000	2.68037900
Al	0.00000000	-1.87229500	0.88145000
Al	0.00000000	-1.25682800	-1.45993900
O	0.00000000	0.00000000	-2.64602000

2a

C	0.00000000	0.33466600	0.00000000
Al	0.61945200	2.23015400	0.00000000
Al	2.01280800	0.23051900	0.00000000
Al	0.43431300	-1.67902900	0.00000000
Al	-1.75864200	-0.58578700	0.00000000
Al	-1.89608200	1.95436900	0.00000000
O	-1.18677500	-2.23792700	0.00000000
O	2.14252000	-1.50719100	0.00000000

2a'

Al	0.00000000	0.00000000	2.76987900
Al	0.00000000	1.76459100	0.76188300
Al	0.00000000	1.24706000	-1.66687200
Al	0.00000000	-1.24706000	-1.66687200
Al	0.00000000	-1.76459100	0.76188300
C	0.00000000	0.00000000	-0.11703800
O	0.00000000	2.72880400	-0.73603000
O	0.00000000	-2.72880400	-0.73603000

3a

C	0.00000000	0.00000000	0.31635300

Al	0.00000000	0.00000000	2.53727400
Al	0.00000000	1.86392900	1.04565500
Al	0.00000000	1.23327500	-1.31921600
Al	0.00000000	-1.23327500	-1.31921600
Al	0.00000000	-1.86392900	1.04565500
O	0.00000000	-2.72541200	-0.47421300
O	0.00000000	0.00000000	-2.52283700
O	0.00000000	2.72541200	-0.47421300

3a'

C	0.00000000	0.00000000	-0.14205100
Al	0.00000000	1.23151200	-1.76655100
Al	0.00000000	-1.23151200	-1.76655100
Al	0.00000000	-2.02263300	0.45085800
Al	0.00000000	0.00000000	1.88153200
Al	0.00000000	2.02263300	0.45085800
O	0.00000000	1.69349100	2.15336400
O	0.00000000	-1.69349100	2.15336400
O	0.00000000	0.00000000	-2.98168000

4a

C	0.00000000	0.00000000	-0.21060800
Al	0.11903400	1.16569600	-1.90823600
Al	-0.10250900	1.95476100	0.40868500
Al	0.00000000	0.00000000	1.88417300
Al	0.10250900	-1.95476100	0.40868500
Al	-0.11903400	-1.16569600	-1.90823600
O	0.00000000	-2.70802100	-1.12477900
O	0.09489700	-1.69864300	2.10963600
O	-0.09489700	1.69864300	2.10963600
O	0.00000000	2.70802100	-1.12477900

5a

Al	0.00000000	2.06837100	0.00000000
Al	-1.21575800	-1.67334700	0.00000000
Al	1.21575800	-1.67334700	0.00000000
Al	1.96713800	0.63916200	0.00000000
C	0.00000000	0.00000000	0.00000000
O	-1.69484000	2.33274800	0.00000000
O	1.69484000	2.33274800	0.00000000
O	2.74230900	-0.89103000	0.00000000
O	0.00000000	-2.88343500	0.00000000
O	-2.74230900	-0.89103000	0.00000000
Al	-1.96713800	0.63916200	0.00000000

6a

Al	-0.31211800	1.73260500	1.23294300
Al	-0.03116300	-0.74959500	-1.90024100
Al	0.70895000	-2.18515000	0.00000000
Al	-0.03116300	-0.74959500	1.90024100
C	0.29706600	-0.17809500	0.00000000
O	-1.16440500	2.58789900	0.00000000
O	-0.31211800	0.76860400	2.65209100
O	0.27350400	-2.43010900	1.65385000
O	0.27350400	-2.43010900	-1.65385000
O	-0.31211800	0.76860400	-2.65209100
Al	-0.31211800	1.73260500	-1.23294300
O	0.98245200	1.22476800	0.00000000

MP2/aug-cc-pVTZ-optimized structures.

0

C	0.00000000	0.00000000	0.00000000
Al	0.00000000	2.13711100	0.00000000
Al	2.03251400	0.66040400	0.00000000
Al	1.25616300	-1.72895900	0.00000000
Al	-1.25616300	-1.72895900	0.00000000
Al	-2.03251400	0.66040400	0.00000000

1a

C	0.00000000	0.00000000	0.23947100
Al	0.00000000	1.27099300	-1.48194600
Al	0.00000000	1.90601600	0.88529500
Al	0.00000000	0.00000000	2.72321000
Al	0.00000000	-1.90601600	0.88529500
Al	0.00000000	-1.27099300	-1.48194600
O	0.00000000	0.00000000	-2.66570300

2a

C	0.00000000	0.00000000	-0.36313000
Al	0.00000000	1.23875800	-2.16615800
Al	0.00000000	1.94715200	0.19593600
Al	0.00000000	0.00000000	1.72838300
Al	0.00000000	-1.94715200	0.19593600
Al	0.00000000	-1.23875800	-2.16615800
O	0.00000000	-1.71536400	1.93347400
O	0.00000000	1.71536400	1.93347400

2a'

Al	0.00000000	0.00000000	2.70587500
Al	0.00000000	1.77494600	0.76680700
Al	0.00000000	1.24857800	-1.65187800
Al	0.00000000	-1.24857800	-1.65187800
Al	0.00000000	-1.77494600	0.76680700
C	0.00000000	0.00000000	-0.09680700
O	0.00000000	2.72358300	-0.72398000
O	0.00000000	-2.72358300	-0.72398000

3a

C	0.00000000	0.00000000	0.32637200
Al	0.00000000	0.00000000	2.52610800
Al	0.00000000	1.88756400	1.05689600
Al	0.00000000	1.24595800	-1.32465600
Al	0.00000000	-1.24595800	-1.32465600
Al	0.00000000	-1.88756400	1.05689600
O	0.00000000	-2.74850800	-0.47433200
O	0.00000000	0.00000000	-2.53082000
O	0.00000000	2.74850800	-0.47433200

3a'

C	0.00000000	0.00000000	-0.14282000
Al	0.00000000	1.23659100	-1.78094700
Al	0.00000000	-1.23659100	-1.78094700
Al	0.00000000	-2.03089300	0.45592900
Al	0.00000000	0.00000000	1.89592100
Al	0.00000000	2.03089300	0.45592900
O	0.00000000	1.70625500	2.16966300
O	0.00000000	-1.70625500	2.16966300
O	0.00000000	0.00000000	-3.00677400

4a

C	0.00000000	0.00000000	-0.21227900
Al	0.11754500	1.17374100	-1.91711800
Al	-0.10400600	1.96763700	0.41008800
Al	0.00000000	0.00000000	1.89467400
Al	0.10400600	-1.96763700	0.41008800
Al	-0.11754500	-1.17374100	-1.91711800
O	0.00000000	-2.72815800	-1.13382700
O	0.09889800	-1.70981100	2.12293100
O	-0.09889800	1.70981100	2.12293100
O	0.00000000	2.72815800	-1.13382700

5a

Al	-0.64274100	1.97815500	0.00000000
Al	-0.64274100	-1.97815400	0.00000000
Al	1.68271900	-1.22256700	0.00000000
Al	1.68271900	1.22256700	0.00000000
C	0.00000000	0.00000000	0.00000000
O	-2.34841700	1.70622500	0.00000000
O	0.89701500	2.76072900	0.00000000
O	2.90280300	0.00000000	0.00000000
O	0.89701500	-2.76072900	0.00000000
O	-2.34841700	-1.70622500	0.00000000
Al	-2.07995500	0.00000000	0.00000000

6a

Al	-0.27642400	1.72443900	1.23236900
Al	-0.04694300	-0.74653000	-1.93032000
Al	0.63121100	-2.19200300	0.00000000
Al	-0.04694300	-0.74653000	1.93032000
C	0.24661900	-0.16516400	0.00000000
O	-1.10481500	2.62242600	0.00000000
O	-0.27642400	0.78620400	2.68455900
O	0.23136500	-2.44104700	1.67033800
O	0.23136500	-2.44104700	-1.67033800
O	-0.27642400	0.78620400	-2.68455900
Al	-0.27642400	1.72443900	-1.23236900
O	1.03519100	1.19493500	0.00000000

TPSS/aug-cc-pVTZ-optimized structures

0

C	0.00000000	0.00000000	0.00000000
Al	0.00000000	2.10982200	0.00000000
Al	-2.00656000	0.65197100	0.00000000
Al	1.24012200	-1.70688100	0.00000000
Al	2.00656000	0.65197100	0.00000000
Al	-1.24012200	-1.70688100	0.00000000

1a

C	0.00000000	0.00000000	0.25730700
Al	0.00000000	1.24384800	-1.41565500
Al	0.00000000	1.93456400	0.90754400
Al	0.00000000	0.00000000	2.52202200

Al	0.00000000	-1.93456400	0.90754400
Al	0.00000000	-1.24384800	-1.41565500
O	0.00000000	0.00000000	-2.63990500

2a

C	0.00000000	0.36099700	0.00000000
Al	1.23055700	2.15406400	0.00000000
Al	1.93843400	-0.19088000	0.00000000
Al	0.00088600	-1.71271900	0.00000000
Al	-1.93779200	-0.19229600	0.00000000
Al	-1.23327100	2.15438600	0.00000000
O	-1.71554600	-1.93371500	0.00000000
O	1.71747300	-1.93243500	0.00000000

2a'

Al	0.00000000	0.00000000	2.68680700
Al	0.00000000	1.76598300	0.76673500
Al	0.00000000	1.23939900	-1.64469200
Al	0.00000000	-1.23939900	-1.64469200
Al	0.00000000	-1.76598300	0.76673500
C	0.00000000	0.00000000	-0.08909700
O	0.00000000	2.72154900	-0.72293900
O	0.00000000	-2.72154900	-0.72293900

3a

C	0.00000000	0.00000000	0.32052200
Al	0.00000000	0.00000000	2.54599300
Al	0.00000000	1.87464700	1.05007700
Al	0.00000000	1.23861200	-1.32161700
Al	0.00000000	-1.23861200	-1.32161700
Al	0.00000000	-1.87464700	1.05007700
O	0.00000000	-2.74842800	-0.47799100
O	0.00000000	0.00000000	-2.53914200
O	0.00000000	2.74842800	-0.47799100

3a'

C	0.00000000	0.00000000	-0.14220800
Al	0.00000000	1.23443400	-1.77711100
Al	0.00000000	-1.23443400	-1.77711100
Al	0.00000000	-2.02723300	0.45423400
Al	0.00000000	0.00000000	1.88997200
Al	0.00000000	2.02723300	0.45423400
O	0.00000000	1.70590300	2.17185600
O	0.00000000	-1.70590300	2.17185600

O	0.00000000	0.00000000	-3.00890900

4a

C	0.00000000	0.00000000	-0.21303300
Al	0.11858700	1.17231800	-1.91408200
Al	-0.10081900	1.96258500	0.40920500
Al	0.00000000	0.00000000	1.88839500
Al	0.10081900	-1.96258500	0.40920500
Al	-0.11858700	-1.17231800	-1.91408200
O	0.00000000	-2.73044000	-1.13307400
O	0.09448600	-1.71137200	2.12406600
O	-0.09448600	1.71137200	2.12406600
O	0.00000000	2.73044000	-1.13307400

5a

Al	2.07389400	0.00000000	0.00000000
Al	-1.67783500	1.21901800	0.00000000
Al	-1.67783500	-1.21901800	0.00000000
Al	0.64088000	-1.97243100	0.00000000
C	0.00000100	0.00000000	0.00000000
O	2.34957300	1.70704100	0.00000000
O	2.34957300	-1.70704100	0.00000000
O	-0.89745100	-2.76207100	0.00000000
O	-2.90422000	0.00000000	0.00000000
O	-0.89745100	2.76207100	0.00000000
Al	0.64088000	1.97243100	0.00000000

6a

Al	-0.27107300	1.71693200	1.22731200
Al	-0.03955600	-0.74182900	-1.92495600
Al	0.62515100	-2.19456100	0.00000000
Al	-0.03955600	-0.74182900	1.92495600
C	0.26784900	-0.16020300	0.00000000
O	-1.11903800	2.60872100	0.00000000
O	-0.27107300	0.78738200	2.68892900
O	0.19749800	-2.44294900	1.66649900
O	0.19749800	-2.44294900	-1.66649900
O	-0.27107300	0.78738200	-2.68892900
Al	-0.27107300	1.71693200	-1.22731200
O	1.05897200	1.21964400	0.00000000

Cartesian coordinates of structures shown in Fig. 4.

B3LYP/aug-cc-pVTZ-optimized geometries.

1a

C	0.00000000	0.00000000	0.22732200
Al	0.00000000	1.25682800	-1.45993900
Al	0.00000000	1.87229500	0.88145000
Al	0.00000000	0.00000000	2.68037900
Al	0.00000000	-1.87229500	0.88145000
Al	0.00000000	-1.25682800	-1.45993900
O	0.00000000	0.00000000	-2.64602000

1b

C	1.22555700	0.00049500	-0.00013100
Al	-0.62053400	0.00017200	0.00002600
Al	1.83374500	-0.87694500	1.80030100
Al	1.83286500	-1.12161000	-1.65926100
Al	1.83365900	1.99811100	-0.14127300
Al	-4.04502700	0.00004300	0.00019900
O	-2.27556700	0.00000000	0.00010900

1c

C	0.00000000	0.00000000	-1.13602800
Al	0.00000000	1.29947300	0.31442200
Al	0.00000000	-1.29947300	0.31442200
Al	-1.74328300	0.00000000	-2.30388900
Al	1.74328300	0.00000000	-2.30388900
Al	0.00000000	0.00000000	3.49190800
O	0.00000000	0.00000000	1.64343900

1d

C	0.00000000	0.00000000	-0.74427300
Al	0.00000000	1.73159700	-1.58986500
Al	0.00000000	0.00000000	-3.73512600
Al	0.00000000	-1.73159700	-1.58986500
Al	0.00000000	0.00000000	4.49669300
Al	0.00000000	0.00000000	1.07791900
O	0.00000000	0.00000000	2.73610200

1e

C	-0.44787000	0.93312400	-0.00002400
Al	-4.53914300	-1.60500000	0.00004200

Al	-0.45566900	2.90326800	-0.00003600
Al	1.14869000	0.06905700	-0.00000500
Al	-1.90458500	-0.21114600	-0.00003400
Al	4.30989600	-1.22659100	0.00003800
O	2.67721900	-0.58542400	0.00001100

2a

C	0.00000000	0.33466600	0.00000000
Al	0.61945200	2.23015400	0.00000000
Al	2.01280800	0.23051900	0.00000000
Al	0.43431300	-1.67902900	0.00000000
Al	-1.75864200	-0.58578700	0.00000000
Al	-1.89608200	1.95436900	0.00000000
O	-1.18677500	-2.23792700	0.00000000
O	2.14252000	-1.50719100	0.00000000

2b

C	0.00000000	0.00000000	1.05988700
Al	0.00000000	1.51733500	0.04669000
Al	0.00000000	-1.51733500	0.04669000
Al	0.00000000	0.00000000	3.03137500
Al	0.00000000	-4.61635800	-1.39837600
Al	0.00000000	4.61635800	-1.39837600
O	0.00000000	-3.01508400	-0.66396000
O	0.00000000	3.01508400	-0.66396000

2c

C	0.00000000	0.00000000	-0.03590700
Al	0.00000000	1.30830600	-1.41149800
Al	0.00000000	0.00000000	-4.57768700
Al	0.00000000	0.00000000	1.78614800
Al	0.00000000	-1.30830600	-1.41149800
Al	0.00000000	0.00000000	5.20380300
O	0.00000000	0.00000000	3.44115700
O	0.00000000	0.00000000	-2.74678900

2d

C	1.90923000	0.01889900	0.00000000
Al	3.24018700	1.34075800	0.00000000
Al	1.42197400	-1.79416200	0.00000000
Al	-2.47617800	2.64731600	0.00000000
Al	0.00000000	0.30361600	0.00000000
Al	-2.02286800	-2.39479700	0.00000000
O	-0.40400400	-1.54774400	0.00000000

O	-1.29298000	1.36663300	0.00000000

2e

C	1.83684200	0.12823600	0.00000000
Al	0.00000000	0.61142300	0.00000000
Al	-2.30564800	3.11052500	0.00000000
Al	1.23379800	-1.67154800	0.00000000
Al	-2.25284400	-1.88515700	0.00000000
Al	3.57953000	-0.50865900	0.00000000
O	-0.53100400	-1.24469500	0.00000000
O	-1.26073700	1.70656800	0.00000000

3a

C	0.00000000	0.00000000	0.31635300
Al	0.00000000	0.00000000	2.53727400
Al	0.00000000	1.86392900	1.04565500
Al	0.00000000	1.23327500	-1.31921600
Al	0.00000000	-1.23327500	-1.31921600
Al	0.00000000	-1.86392900	1.04565500
O	0.00000000	-2.72541200	-0.47421300
O	0.00000000	0.00000000	-2.52283700
O	0.00000000	2.72541200	-0.47421300

3b

C	-2.59241900	-0.73568000	0.00000000
Al	-1.05669600	-1.80844500	0.00000000
Al	4.62230800	0.77600600	0.00000000
Al	-4.17075700	0.25224800	0.00000000
Al	1.29340400	0.08064400	0.00000000
Al	-1.65400400	0.95371500	0.00000000
O	2.92334900	0.41693200	0.00000000
O	0.59030000	-1.51546700	0.00000000
O	0.00000000	1.23727200	0.00000000

3c

C	-2.68426100	0.46821200	0.00305600
Al	1.41166900	0.29125800	0.00122500
Al	-1.73293000	-1.21087700	0.00396000
Al	-4.25317300	-0.52902600	-0.00600000
Al	4.67624700	-0.66902400	-0.00374600
Al	-1.01042700	1.31839000	0.00080700
O	0.60734900	1.83167400	-0.00117000
O	-0.09827100	-0.64286100	0.00367600
O	2.98061500	-0.24114400	0.00130400

3d

C	-2.74162700	0.19292700	0.00000000
Al	-4.31377700	-0.82736900	0.00000000
Al	-1.56183800	1.70040800	0.00000000
Al	1.40133700	-0.19313100	0.00000000
Al	4.75474100	0.38434800	0.00000000
Al	-1.11769800	-0.81870200	0.00000000
O	0.00000000	0.91173800	0.00000000
O	3.02224000	0.15186600	0.00000000
O	0.39448600	-1.60732500	0.00000000

3e

C	1.55185800	-0.32184400	0.00000000
Al	0.00000000	0.80367800	0.00000000
Al	3.36299900	-0.12473600	0.00000000
Al	-0.93189200	4.08109000	0.00000000
Al	-2.13159000	-2.07756500	0.00000000
Al	0.39044900	-1.76605700	0.00000000
O	-1.15055700	-0.57721200	0.00000000
O	-0.70167900	-3.08646400	0.00000000
O	-0.43285400	2.41589300	0.00000000

4a

C	0.00000000	0.00000000	-0.21060800
Al	0.11903400	1.16569600	-1.90823600
Al	-0.10250900	1.95476100	0.40868500
Al	0.00000000	0.00000000	1.88417300
Al	0.10250900	-1.95476100	0.40868500
Al	-0.11903400	-1.16569600	-1.90823600
O	0.00000000	-2.70802100	-1.12477900
O	0.09489700	-1.69864300	2.10963600
O	-0.09489700	1.69864300	2.10963600
O	0.00000000	2.70802100	-1.12477900

4b

C	0.03440900	2.25459300	0.00000000
Al	0.24480000	0.03900500	0.00000000
Al	-0.86085100	-0.66586600	-3.08436200
Al	3.65064300	-0.21202900	0.00000000
Al	-2.33485400	-1.06911800	0.00000000
Al	-0.86085100	-0.66586600	3.08436200
O	-0.86085100	-0.44755300	1.28787800
O	-0.86085100	-0.44755300	-1.28787800

O	1.92034400	0.01600800	0.00000000
O	0.03735800	3.37069700	0.00000000

4c

C	0.24920200	3.31695200	0.00000000
Al	2.31158900	-1.08946700	0.00000000
Al	-0.28481700	-0.03790000	0.00000000
Al	-3.69262300	0.09019600	0.00000000
Al	0.82163200	-0.64680800	-3.09534000
Al	0.82163200	-0.64680800	3.09534000
O	0.82163200	-0.49004400	-1.28743200
O	0.15238000	2.18668400	0.00000000
O	0.82163200	-0.49004400	1.28743200
O	-1.94584500	0.09322000	0.00000000

4d

C	-2.11604200	3.65479100	0.00000000
Al	0.73276200	2.53407600	0.00000000
Al	3.91512900	-1.87860300	0.00000000
Al	-1.91765300	0.22083000	0.00000000
Al	-1.52333000	-3.27857900	0.00000000
Al	0.68725700	-0.76766400	0.00000000
O	2.25860300	-1.30197900	0.00000000
O	-2.90010800	4.45796300	0.00000000
O	-0.84948300	-1.59025800	0.00000000
O	0.00000000	0.84433400	0.00000000

4e

C	1.68066900	2.06162300	0.60585300
Al	-1.36379300	0.21195400	-0.61827600
Al	-0.47669300	-1.49122000	2.27800200
Al	4.04279000	-1.24014600	-1.10773100
Al	-4.77045900	0.03984700	-0.74301600
Al	1.02484700	0.18101600	-0.37969900
O	2.54696600	-0.47814800	-0.63127100
O	-3.02817700	0.07754700	-0.57794800
O	-0.27752100	-0.49408600	0.76045300
O	2.00610700	3.08361200	0.92179600

5a

Al	0.00000000	2.06837100	0.00000000
Al	-1.21575800	-1.67334700	0.00000000
Al	1.21575800	-1.67334700	0.00000000
Al	1.96713800	0.63916200	0.00000000

C	0.00000000	0.00000000	0.00000000
O	-1.69484000	2.33274800	0.00000000
O	1.69484000	2.33274800	0.00000000
O	2.74230900	-0.89103000	0.00000000
O	0.00000000	-2.88343500	0.00000000
O	-2.74230900	-0.89103000	0.00000000
Al	-1.96713800	0.63916200	0.00000000

5b

C	-1.71372800	1.92359000	0.95894400
Al	1.46043500	0.21654500	-0.42775800
Al	-4.05400500	-1.16625900	-1.15693200
Al	0.31378500	-1.93517600	1.94194300
Al	4.85637600	0.03971600	-0.50431500
Al	-1.07494300	0.25065100	-0.32061500
O	-2.11943300	2.78836300	1.53529200
O	0.18215800	1.00253200	-1.24081600
O	3.10899500	0.04761100	-0.35723400
O	0.25230400	-0.62909100	0.67579000
O	-2.57890600	-0.43601000	-0.57226600

5c

C	-1.86889600	-2.40416000	2.13372200
Al	0.26483100	2.33164000	1.44367000
Al	1.44884800	-0.28731700	-0.39376600
Al	-1.08069800	-0.29550500	-0.30398500
Al	4.84609100	-0.12975400	-0.47422600
Al	-4.20859500	0.68629200	-1.19884000
O	-1.52397900	-1.61270600	1.39656600
O	-2.63460100	0.22368300	-0.59605300
O	3.09638100	-0.10763600	-0.34680000
O	0.22613400	0.78919200	0.47237300
O	0.17321200	-1.23561700	-1.01976400

5d

C	1.85827200	2.55047900	0.00000000
Al	0.12137300	-3.29292700	-2.95118600
Al	0.12137300	-3.29292700	2.95118600
Al	-0.14245800	1.75019000	0.00000000
Al	0.11273600	-1.60750500	0.00000000
Al	-2.37737200	4.33076000	0.00000000
O	0.12137300	-2.33313200	-1.51424800
O	0.11374800	0.13439200	0.00000000
O	2.88937400	2.97111500	0.00000000

O	-1.12250900	3.08056400	0.00000000
O	0.12137300	-2.33313200	1.51424800

5e

C	2.04131100	1.35276800	-1.61986500
Al	-4.81521300	-1.14120500	-0.83037400
Al	1.37858800	-0.07000900	-0.10829900
Al	-1.82689500	0.07289200	0.24754200
Al	4.13280200	-1.99179800	0.49220000
Al	0.08888200	1.57201800	1.80562700
O	2.79106300	-0.91376000	0.15399900
O	-1.53493700	1.17741000	1.54564000
O	-0.26005300	-0.28448300	-0.41244000
O	2.43810300	2.07324900	-2.37304400
O	-3.27217200	-0.53507700	-0.31013800

6a

Al	-0.31211800	1.73260500	1.23294300
Al	-0.03116300	-0.74959500	-1.90024100
Al	0.70895000	-2.18515000	0.00000000
Al	-0.03116300	-0.74959500	1.90024100
C	0.29706600	-0.17809500	0.00000000
O	-1.16440500	2.58789900	0.00000000
O	-0.31211800	0.76860400	2.65209100
O	0.27350400	-2.43010900	1.65385000
O	0.27350400	-2.43010900	-1.65385000
O	-0.31211800	0.76860400	-2.65209100
Al	-0.31211800	1.73260500	-1.23294300
O	0.98245200	1.22476800	0.00000000

6b

C	3.58968700	0.43480900	0.00000000
Al	-2.64055500	0.23092800	4.16180500
Al	1.58178300	-0.39493600	0.00000000
Al	-0.26874400	-0.10669400	-1.74335300
Al	-0.26874400	-0.10669400	1.74335300
Al	-2.64055500	0.23092800	-4.16180500
O	-0.27470500	0.27062400	0.00000000
O	-1.45582500	0.07368900	2.88485200
O	-1.45582500	0.07368900	-2.88485200
O	1.37514200	-0.67074700	-1.67424800
O	4.62863000	0.83539900	0.00000000
O	1.37514200	-0.67074700	1.67424800

6c

C	-2.16137700	-0.46328100	1.97287800
Al	0.21289800	-1.89113000	-0.74456900
Al	4.63401400	1.82334000	0.51102100
Al	-1.55127500	-0.19665700	-0.11324200
Al	2.04312500	-0.27197700	-0.18539600
Al	-3.61176600	2.33084600	-1.09373800
O	-2.57770800	-0.53351900	3.00532800
O	-1.47127800	-1.86739900	-0.70194000
O	1.90529400	-1.90324100	-0.82070400
O	0.26646100	-0.13124600	-0.03038300
O	3.25931600	0.78808400	0.18193900
O	-2.56741900	1.07884500	-0.47177300

6d

C	4.58271400	0.81659400	0.00000000
Al	-2.60295500	0.19559500	4.18693500
Al	1.59651600	-0.34858300	0.00000000
Al	-0.24304500	-0.09560100	-1.75094500
Al	-0.24304500	-0.09560100	1.75094500
Al	-2.60295500	0.19559500	-4.18693500
O	-1.42516900	0.05971700	2.90039900
O	3.50077200	0.46331300	0.00000000
O	-1.42516900	0.05971700	-2.90039900
O	-0.27566100	0.24687000	0.00000000
O	1.42167800	-0.60029800	1.67580600
O	1.42167800	-0.60029800	-1.67580600

6e

C	2.36717500	-0.59479900	3.02146700
Al	-4.61123000	1.87120400	0.40756900
Al	1.56110200	-0.18308100	-0.14139100
Al	-0.19710500	-1.90907700	-0.67828600
Al	-2.02565000	-0.26031400	-0.19369300
Al	3.74788900	2.30055900	-0.92215600
O	-1.88950300	-1.92505800	-0.73653600
O	2.62038600	1.06539800	-0.42366700
O	-0.24724200	-0.10717700	-0.06803900
O	1.48822700	-1.87547700	-0.64198400
O	1.97118800	-0.48472800	1.96289500
O	-3.24032100	0.81679500	0.12415900

TPSS/aug-cc-pVTZ-optimized geometries

1a

C	0.00000000	0.00000000	0.25730700
Al	0.00000000	1.24384800	-1.41565500
Al	0.00000000	1.93456400	0.90754400
Al	0.00000000	0.00000000	2.52202200
Al	0.00000000	-1.93456400	0.90754400
Al	0.00000000	-1.24384800	-1.41565500
O	0.00000000	0.00000000	-2.63990500

1b

C	1.25928500	0.00011600	0.00002500
Al	-0.59884700	0.00000900	0.00007400
Al	1.81705100	-1.09744800	1.69102700
Al	1.81655500	-0.91592000	-1.79595400
Al	1.81600500	2.01362300	0.10471900
Al	-4.03882500	-0.00023100	0.00005400
O	-2.26386300	-0.00014000	0.00011200

1c

C	0.00000000	0.00000000	-1.15009200
Al	0.00000000	1.30497500	0.30253200
Al	0.00000000	-1.30497500	0.30253200
Al	-1.75708200	0.00000000	-2.28929800
Al	1.75708200	0.00000000	-2.28929800
Al	0.00000000	0.00000000	3.49479100
O	0.00000000	0.00000000	1.64052400

1d

C	0.00000000	0.00000000	-0.79785600
Al	0.00000000	1.77221500	-1.60016200
Al	0.00000000	0.00000000	-3.60199400
Al	0.00000000	-1.77221500	-1.60016200
Al	0.00000000	0.00000000	4.47034200
Al	0.00000000	0.00000000	1.03607700
O	0.00000000	0.00000000	2.70422700

1e

C	0.46589000	0.99162600	0.00001800
Al	4.47440300	-1.64457400	-0.00002300
Al	0.46984800	2.95678700	0.00005100
Al	-1.11264000	0.06982700	0.00000000
Al	1.86865500	-0.23603300	0.00000100

Al	-4.28511700	-1.23867300	-0.00002900
O	-2.64903400	-0.59313700	-0.00001300

2a

C	0.00000000	0.36099700	0.00000000
Al	1.23055700	2.15406400	0.00000000
Al	1.93843400	-0.19088000	0.00000000
Al	0.00088600	-1.71271900	0.00000000
Al	-1.93779200	-0.19229600	0.00000000
Al	-1.23327100	2.15438600	0.00000000
O	-1.71554600	-1.93371500	0.00000000
O	1.71747300	-1.93243500	0.00000000

2b

C	0.00000000	0.00000000	1.13708300
Al	0.00000000	1.48059800	0.04598200
Al	0.00000000	-1.48059800	0.04598200
Al	0.00000000	0.00000000	3.09806600
Al	0.00000000	-4.57871800	-1.43508100
Al	0.00000000	4.57871800	-1.43508100
O	0.00000000	-2.98107300	-0.68629900
O	0.00000000	2.98107300	-0.68629900

2c

C	0.00000000	0.00000000	-0.03924200
Al	0.00000000	1.31280500	-1.41596900
Al	0.00000000	0.00000000	-4.59690000
Al	0.00000000	0.00000000	1.79247000
Al	0.00000000	-1.31280500	-1.41596900
Al	0.00000000	0.00000000	5.22537300
O	0.00000000	0.00000000	3.45823200
O	0.00000000	0.00000000	-2.76093600

2d

C	1.94207100	0.40912900	0.00000000
Al	2.61225800	2.14763700	0.00000000
Al	1.84592100	-1.47860900	0.00000000
Al	-2.97105400	1.98379200	0.00000000
Al	0.00000000	0.27855400	0.00000000
Al	-1.44620500	-2.75019800	0.00000000
O	-0.00601500	-1.61942800	0.00000000
O	-1.51703300	1.01817200	0.00000000

2e

C	1.86064900	0.21219100	0.00000000
Al	0.00000000	0.62134800	0.00000000
Al	-2.46023800	2.98300300	0.00000000
Al	1.32504400	-1.62547200	0.00000000
Al	-2.20867900	-1.84386200	0.00000000
Al	3.60299200	-0.45156100	0.00000000
O	-0.46012800	-1.26223800	0.00000000
O	-1.35642700	1.61747700	0.00000000

3a

C	0.00000000	0.00000000	0.32052200
Al	0.00000000	0.00000000	2.54599300
Al	0.00000000	1.87464700	1.05007700
Al	0.00000000	1.23861200	-1.32161700
Al	0.00000000	-1.23861200	-1.32161700
Al	0.00000000	-1.87464700	1.05007700
O	0.00000000	-2.74842800	-0.47799100
O	0.00000000	0.00000000	-2.53914200
O	0.00000000	2.74842800	-0.47799100

3b

C	-2.60914800	-0.75774400	0.00000000
Al	-1.05726000	-1.82279100	0.00000000
Al	4.62032700	0.78396600	0.00000000
Al	-4.15109200	0.29935400	0.00000000
Al	1.28279800	0.07133900	0.00000000
Al	-1.66272800	0.94346500	0.00000000
O	2.92367600	0.41485300	0.00000000
O	0.60611100	-1.54388800	0.00000000
O	0.00000000	1.24992700	0.00000000

3c

C	2.70268000	0.49465500	-0.00446500
Al	-1.42120300	0.31312200	-0.00041700
Al	1.76311600	-1.20446800	-0.00409800
Al	4.24366200	-0.55847900	0.00708300
Al	-4.68294500	-0.70519100	0.00229700
Al	0.99810700	1.30898200	-0.00157700
O	-0.62216400	1.86665000	0.00153600
O	0.11848700	-0.60627100	-0.00405600
O	-2.98703300	-0.25656500	0.00052800

3d

C	-2.79254900	0.40071800	0.00000000

Al	-4.09687800	-0.92271100	0.00000000
Al	-1.51777100	1.84421500	0.00000000
Al	1.35319200	-0.23163000	0.00000000
Al	4.74010600	0.21469700	0.00000000
Al	-1.20307400	-0.71937700	0.00000000
O	0.00000000	0.94893600	0.00000000
O	2.99671000	0.05163200	0.00000000
O	0.27489100	-1.60204500	0.00000000

3e

C	1.56095500	-0.30175100	0.00000000
Al	0.00000000	0.81613000	0.00000000
Al	3.38532500	-0.18233600	0.00000000
Al	-0.94489600	4.10181000	0.00000000
Al	-2.13546200	-2.08606400	0.00000000
Al	0.39023400	-1.75529000	0.00000000
O	-1.16216600	-0.56613400	0.00000000
O	-0.69424200	-3.09917000	0.00000000
O	-0.44400900	2.43846100	0.00000000

4a

C	0.00000000	0.00000000	-0.21303300
Al	0.11858700	1.17231800	-1.91408200
Al	-0.10081900	1.96258500	0.40920500
Al	0.00000000	0.00000000	1.88839500
Al	0.10081900	-1.96258500	0.40920500
Al	-0.11858700	-1.17231800	-1.91408200
O	0.00000000	-2.73044000	-1.13307400
O	0.09448600	-1.71137200	2.12406600
O	-0.09448600	1.71137200	2.12406600
O	0.00000000	2.73044000	-1.13307400

4b

C	0.57085500	2.16599400	0.00000000
Al	-0.22606000	0.14357800	0.00000000
Al	0.69636800	-0.93746500	3.08420300
Al	-3.58251000	0.84586300	0.00000000
Al	1.91000700	-1.68102400	0.00000000
Al	0.69636800	-0.93746500	-3.08420300
O	0.69636800	-0.66399900	-1.28777300
O	0.69636800	-0.66399900	1.28777300
O	-1.84575000	0.61577000	0.00000000
O	0.84684200	3.25831600	0.00000000

4c

C	-1.11289400	3.13369600	0.00000000
Al	-1.90759900	-1.66086100	0.00000000
Al	0.28677900	0.08263900	0.00000000
Al	3.56642900	1.06621200	0.00000000
Al	-0.66254400	-0.88546700	3.09788700
Al	-0.66254400	-0.88546700	-3.09788700
O	-0.66254400	-0.67272400	1.28831900
O	-0.71381400	2.06044900	0.00000000
O	-0.66254400	-0.67272400	-1.28831900
O	1.86522500	0.64451300	0.00000000

4d

C	-1.98085200	2.95724500	0.00000000
Al	0.40969700	2.74024200	0.00000000
Al	3.98782900	-1.74859300	0.00000000
Al	-1.84368000	0.32973500	0.00000000
Al	-1.53712100	-3.18335100	0.00000000
Al	0.73048500	-0.68370600	0.00000000
O	2.30780300	-1.22243300	0.00000000
O	-2.83085500	3.72371000	0.00000000
O	-0.83052500	-1.50154000	0.00000000
O	0.00000000	0.91905000	0.00000000

4e

C	1.60526600	2.01286500	0.73883700
Al	-1.35246100	0.25471900	-0.58711200
Al	-0.45459100	-1.68371300	2.17413000
Al	4.07690600	-1.13502100	-1.19078500
Al	-4.76926000	0.06185300	-0.77386400
Al	1.05205600	0.23067700	-0.32855800
O	2.58157600	-0.41139900	-0.64268900
O	-3.02501800	0.09400700	-0.57557100
O	-0.26733400	-0.56378600	0.73850400
O	1.85877200	3.06269200	1.07318600

5a

Al	2.07389400	0.00000000	0.00000000
Al	-1.67783500	1.21901800	0.00000000
Al	-1.67783500	-1.21901800	0.00000000
Al	0.64088000	-1.97243100	0.00000000
C	0.00000100	0.00000000	0.00000000
O	2.34957300	1.70704100	0.00000000
O	2.34957300	-1.70704100	0.00000000

O	-0.89745100	-2.76207100	0.00000000
O	-2.90422000	0.00000000	0.00000000
O	-0.89745100	2.76207100	0.00000000
Al	0.64088000	1.97243100	0.00000000

5b

C	-1.71645700	1.85350600	1.01750100
Al	1.46679300	0.23697800	-0.42240400
Al	-4.06404900	-1.11617600	-1.21354100
Al	0.32264700	-1.99941000	1.88979800
Al	4.87567500	0.06329700	-0.51020400
Al	-1.07635200	0.26981900	-0.30485300
O	-2.15907800	2.69070500	1.62705400
O	0.18212400	1.05031100	-1.22286300
O	3.12481000	0.06148400	-0.35152600
O	0.25654400	-0.64738500	0.66787500
O	-2.59471900	-0.40882200	-0.57171000

5c

C	-1.87963600	-2.37033800	2.17014600
Al	0.26575800	2.36352600	1.41471700
Al	1.45236900	-0.29923300	-0.38589000
Al	-1.08540100	-0.30608200	-0.28915300
Al	4.86190900	-0.13681100	-0.48598900
Al	-4.21679800	0.66643300	-1.22828700
O	-1.52956900	-1.58336900	1.41487400
O	-2.64477100	0.22411500	-0.59122400
O	3.10915200	-0.11000700	-0.34241200
O	0.22746900	0.7958530	0 0.47764900
O	0.17096000	-1.26656800	-1.00276900

5d

C	-1.81794200	2.60459400	0.00000000
Al	-0.14464600	-3.33396400	2.93159500
Al	-0.14464600	-3.33396400	-2.93159500
Al	0.11904600	1.77682400	0.00000000
Al	-0.14169900	-1.59378100	0.00000000
Al	2.46329600	4.27612300	0.00000000
O	-0.14464600	-2.33008300	1.52075100
O	-0.15369400	0.15079200	0.00000000
O	-2.84596700	3.06610800	0.00000000
O	1.15646200	3.07905800	0.00000000
O	-0.14464600	-2.33008300	-1.52075100

5e

C	-2.11919300	1.30470000	1.57781500
Al	4.82325700	-1.20674800	0.81690500
Al	-1.39671400	-0.02613400	0.05948200
Al	1.85495400	0.11150300	-0.24062100
Al	-4.07845400	-2.07119900	-0.53904200
Al	-0.07010100	1.62512800	-1.63729700
O	-2.79664500	-0.92290600	-0.18939100
O	1.59543600	1.30399900	-1.48725800
O	0.25970700	-0.25973500	0.36664800
O	-2.60177700	1.99595300	2.32512900
O	3.29164300	-0.54873000	0.30494100

6a

Al	-0.27107300	1.71693200	1.22731200
Al	-0.03955600	-0.74182900	-1.92495600
Al	0.62515100	-2.19456100	0.00000000
Al	-0.03955600	-0.74182900	1.92495600
C	0.26784900	-0.16020300	0.00000000
O	-1.11903800	2.60872100	0.00000000
O	-0.27107300	0.78738200	2.68892900
O	0.19749800	-2.44294900	1.66649900
O	0.19749800	-2.44294900	-1.66649900
O	-0.27107300	0.78738200	-2.68892900
Al	-0.27107300	1.71693200	-1.22731200
O	1.05897200	1.21964400	0.00000000

6b

C	3.56321000	0.44504100	0.00000000
Al	-2.64584700	0.23380000	4.17407100
Al	1.58538400	-0.40423900	0.00000000
Al	-0.26050300	-0.10949700	-1.74981000
Al	-0.26050300	-0.10949700	1.74981000
Al	-2.64584700	0.23380000	-4.17407100
O	-0.26236900	0.29139300	0.00000000
O	-1.45969500	0.07533300	2.89283900
O	-1.45969500	0.07533300	-2.89283900
O	1.38731500	-0.69539200	-1.68702700
O	4.60411300	0.86784800	0.00000000
O	1.38731500	-0.69539200	1.68702700

6c

C	-2.16527100	-0.40374000	1.96070000
Al	0.21925400	-1.90865600	-0.70337500

Al	4.66134000	1.83755800	0.47022200
Al	-1.55609000	-0.21119900	-0.09449500
Al	2.05517400	-0.27667300	-0.17694600
Al	-3.63330600	2.28852700	-1.15516200
O	-2.61536100	-0.41330100	2.99304500
O	-1.47815500	-1.89849900	-0.66746600
O	1.92461900	-1.92971700	-0.78648100
O	0.26996400	-0.12631100	-0.01705300
O	3.27794800	0.79905000	0.17001400
O	-2.59291600	1.06105200	-0.46547900

6d

C	4.60683200	0.80351100	0.00000000
Al	-2.61336400	0.18808700	4.20436100
Al	1.59460300	-0.34103200	0.00000000
Al	-0.24126900	-0.09207200	-1.75917300
Al	-0.24126900	-0.09207200	1.75917300
Al	-2.61336400	0.18808700	-4.20436100
O	-1.43515300	0.05971800	2.91183100
O	3.51324100	0.45459100	0.00000000
O	-1.43515300	0.05971800	-2.91183100
O	-0.27877800	0.26469300	0.00000000
O	1.43352300	-0.59961300	1.68965200
O	1.43352300	-0.59961300	-1.68965200

6e

C	2.37532500	-0.61914300	3.02395100
Al	-4.63835600	1.86746000	0.41074800
Al	1.57038500	-0.18261600	-0.13375200
Al	-0.19439100	-1.90471700	-0.68691400
Al	-2.03318500	-0.26096100	-0.19479300
Al	3.76009200	2.31289300	-0.92537400
O	-1.89958000	-1.93150400	-0.75494800
O	2.63738100	1.07551000	-0.40536300
O	-0.24669800	-0.09835500	-0.05642000
O	1.50419000	-1.88121900	-0.65163900
O	1.97556900	-0.49684900	1.95730400
O	-3.25724200	0.81967900	0.12949100