Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

DFT studies on the structure and properties of the carbon aluminum Al_3C cluster, a pseudohalogen superatom

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Table S1 The xyz coordinates in Å for the structures of Al_xC (x=1,2,4,5) calculated at B3LYP/6-311+g(3df) and BP86/6-311+g(3df) levels of theory

B3LYP

$^4C_{\infty V}$ AlC		-280.367981	Hartrees
Atom	x	y	z
Al	0.000000	0.000000	0.621991
C	0.000000	0.000000	-1.347648

BP86

$^4C_{\infty V}$ AlC		-280.363009	Hartrees
Atom	x	y	z
Al	0.000000	0.000000	0.624262
C	0.000000	0.000000	-1.352568

B3LYP

$^3C_{2V}$ Al_2C		-522.873155	Hartrees
Atom	x	y	z
Al	0.000000	1.478064	-0.211871
Al	0.000000	-1.478064	-0.211871
C	0.000000	0.000000	0.918108

BP86

$^3C_{2V}$ Al_2C		-522.877587	Hartrees
Atom	x	y	z
Al	0.000000	1.436635	-0.223372
Al	0.000000	-1.436635	-0.223372
C	0.000000	0.000000	0.967945

B3LYP

^1T_d Al_4C		-1007.875748	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	1.153794	1.153794	1.153794
Al	-1.153794	-1.153794	1.153794
Al	-1.153794	1.153794	-1.153794
Al	1.153794	-1.153794	-1.153794

BP86

^1T_d Al_4C		-1007.877667	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	1.161024	1.161024	1.161024
Al	-1.161024	-1.161024	1.161024
Al	-1.161024	1.161024	-1.161024
Al	1.161024	-1.161024	-1.161024

B3LYP

$^2C_{2V}$ Al_5C		-1250.320357	Hartrees
Atom	x	y	z
Al	0.000000	1.472484	0.688480
Al	0.000000	0.000000	2.998548
Al	0.000000	-1.472484	0.688480
Al	0.000000	1.361819	-2.067036
C	0.000000	0.000000	-0.523110
Al	0.000000	-1.361819	-2.067036

BP86

^2C_s Al_5C		-1250.342254	Hartrees
Atom	x	y	z
Al	-0.147135	0.719768	1.522969
Al	0.629417	2.788137	0.000000
Al	-0.147135	0.719768	-1.522969
Al	-0.147135	-2.010113	1.351678
C	-0.088572	-0.449469	0.000000
Al	-0.147135	-2.010113	-1.351678

Table S2 The xyz coordinates in Å for the structures of Al_3C_x(x=0-5) calculated at B3LYP/6-311+g(3df) and BP86/6-311+g(3df) levels of theory

B3LYP

$^2D_{3h}$ Al_3		-727.281202	Hartrees
Atom	x	y	z
Al	0.000000	1.462229	0.000000
Al	1.266328	-0.731115	0.000000
Al	-1.266328	-0.731115	0.000000

BP86

$^2D_{3h}$ Al_3		-727.295076	Hartrees
Atom	x	y	z
Al	0.000000	1.457267	0.000000
Al	1.262031	-0.728634	0.000000
Al	-1.262031	-0.728634	0.000000

B3LYP

$^2C_{2v}$ Al_3C		-765.393839	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.014735
Al	0.000000	0.000000	1.979011
Al	0.000000	1.566398	-0.992906
Al	0.000000	-1.566398	-0.992906

BP86

$^2C_{2v}$ Al_3C		-765.397605	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.016846
Al	0.000000	0.000000	1.989595
Al	0.000000	1.570501	-0.998685
Al	0.000000	-1.570501	-0.998685

B3LYP

$^2C_{2v}$ Al_3C_2		-803.502321	Hartrees
Atom	x	y	z
C	0.000000	0.628765	-0.775153
C	0.000000	-0.628765	-0.775153
Al	0.000000	2.595873	-0.334718
Al	0.000000	-2.595873	-0.334718
Al	0.000000	0.000000	1.384962

BP86

^2C_s Al_3C_2		-803.502937	Hartrees
Atom	x	y	z
C	0.000000	1.074671	0.000000
C	1.097348	0.429692	0.000000
Al	-1.962106	1.626312	0.000000
Al	2.155152	-1.291223	0.000000
Al	-0.699514	-1.029411	0.000000

B3LYP

$^2C_{2V}$ Al_3C_3		-841.591480	Hartrees
Atom	x	y	z
C	0.000000	1.270498	-0.379476
C	0.000000	0.000000	-0.658344
C	0.000000	-1.270498	-0.379476
Al	0.000000	3.232855	-0.420146
Al	0.000000	-3.232855	-0.420146
Al	0.000000	0.000000	1.494427

BP86

$^2C_2$ Al_3C_3		-841.591943	Hartrees
Atom	x	y	z
C	0.000000	1.281630	-0.777699
C	0.000000	0.000000	-1.089582
C	0.000000	-1.281630	-0.777699
Al	-0.974427	2.705872	0.096697
Al	0.974427	-2.705872	0.096697
Al	0.000000	0.000000	1.027367

B3LYP

BP86

^2C_s Al_3C_4		-879.681961	Hartrees
Atom	x	y	z
C	-0.849699	1.365150	0.000000
C	0.000000	0.426719	0.000000
C	0.978594	-0.490085	0.000000
C	1.874502	-1.345059	0.000000
Al	-2.036142	2.958698	0.000000
Al	3.353910	-2.650240	0.000000
Al	-2.242413	-0.288484	0.000000

^2C_s Al_3C_4		-879.679977	Hartrees
Atom	x	y	z
C	-0.976950	1.287579	0.000000
C	0.000000	0.463528	0.000000
C	1.074052	-0.340610	0.000000
C	2.073385	-1.095761	0.000000
Al	-2.520565	2.564464	0.000000
Al	3.714099	-2.210686	0.000000
Al	-2.195297	-0.499040	0.000000

B3LYP

$^2C_1$ Al_3C_5		-917.707983	Hartrees
Atom	x	y	z
C	-2.228536	-0.016714	0.414929
C	-0.857375	0.064659	0.682655
C	0.418553	-0.092750	0.337420
C	1.656586	-0.267627	0.047396
C	-1.846227	0.459514	1.662257
Al	3.345242	-1.267816	-0.079331
Al	-3.701177	-0.530960	-0.851020
Al	1.674550	1.730891	-0.521029

BP86

$^2C_1$ Al_3C_5		-917.709669	Hartrees
Atom	x	y	z
C	-2.305975	0.087851	0.453680
C	-0.909636	0.164172	0.723766
C	0.354466	-0.074300	0.394856
C	1.601073	-0.313535	0.113642
C	-1.915564	0.692210	1.644182
Al	3.349372	-1.207450	0.029248
Al	-3.646262	-0.626174	-0.879005
Al	1.762569	1.576824	-0.687224

Table S3 The xyz coordinates in Å for the structures of $Al_7(CAl_3)$, Al_7I and Al_7 calculated at M06/TZ2P level of theory

M06/TZ2P

$^2C_{3V}$ $Al_7(CAl_3)$

Atom	x	y	z
Al	4.787473	3.450562	-0.324201
Al	4.288148	1.227679	0.831559
Al	3.106056	2.724828	2.947421
Al	3.687844	4.838747	1.635661
Al	5.523038	3.017764	2.174296
Al	2.310485	3.193730	0.249881
Al	1.806378	0.998213	1.524163
C	0.414144	-0.312499	1.708268
Al	1.106454	-1.588672	3.009934
Al	0.186489	-1.047629	-0.082930
Al	-1.124812	0.705504	2.345661

M06/TZ2P

$^2C_{3V}$ Al_7I

Atom	x	y	z
Al	3.748802	1.774559	1.695678
Al	1.333286	2.605812	1.807899
Al	1.086502	1.869273	-0.995098

Al	3.518936	1.091822	-0.886281
Al	2.792663	3.537268	-0.074268
Al	2.133766	-0.055117	0.932166
Al	-0.314808	0.811893	0.915102
I	-2.603742	-0.085410	1.351574

M06/TZ2P

$^2C_{3V}$ Al_7

Atom	x	y	z
Al	-0.765779	0.348414	-1.517739
Al	0.285711	2.571440	-0.519589
Al	0.619730	-1.191228	1.634153
Al	-1.682481	-1.266586	0.250577
Al	-0.778929	0.912717	1.253848
Al	0.619472	-1.746009	-1.023203
Al	1.702275	0.371247	-0.078049

Table S4 The xyz coordinates in Å for the structures of $K_x(CAl_3)_y$ (x=1-5,y=2-6) calculated at B3LYP/6-311+g(3df) and BP86/6-311+g(3df) levels of theory

B3LYP

$^1D_{3d}$ $K(CAl_3)_2$		-2130.905974	Hartrees
Atom	x	y	z
C	0.000000	0.000000	3.024817
Al	0.000000	1.888266	3.351351
Al	-1.635286	-0.944133	3.351351
Al	1.635286	-0.944133	3.351351
K	0.000000	0.000000	0.000000
Al	1.635286	0.944133	-3.351351
Al	-1.635286	0.944133	-3.351351
Al	0.000000	-1.888266	-3.351351
C	0.000000	0.000000	-3.024817

BP86

$^1D_{3d}$ $K(CAl_3)_2$		-2130.967712	Hartrees
Atom	x	y	z
C	0.000000	0.000000	3.008097
Al	0.000000	1.891757	3.331989
Al	-1.638309	-0.945878	3.331989
Al	1.638309	-0.945878	3.331989
K	0.000000	0.000000	0.000000
Al	1.638309	0.945878	-3.331989
Al	-1.638309	0.945878	-3.331989
Al	0.000000	-1.891757	-3.331989
C	0.000000	0.000000	-3.008097

B3LYP

$^1D_{3h}$ $K_2(CAl_3)_3$		-3496.317899	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	0.000000	1.922643	0.000000
Al	1.665058	-0.961322	0.000000
Al	-1.665058	-0.961322	0.000000

BP86

$^1C_{3h}$ $K_2(CAl_3)_3$		-3496.409339	Hartrees
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	-1.936296	-0.000139	0.000000
Al	0.968027	1.676951	0.000000
Al	0.968269	-1.676812	0.000000

K	0.000000	0.000000	3.348591	K	0.000000	0.000000	3.326438
Al	-1.636602	0.944893	6.621295	Al	-0.950981	-1.647005	6.581757
Al	1.636602	0.944893	6.621295	Al	-0.950858	1.647076	6.581757
Al	0.000000	-1.889785	6.621295	Al	1.901839	-0.000071	6.581757
K	0.000000	0.000000	-3.348591	K	0.000000	0.000000	-3.326438
Al	1.636602	0.944893	-6.621295	Al	-0.950858	1.647076	-6.581757
Al	0.000000	-1.889785	-6.621295	Al	1.901839	-0.000071	-6.581757
Al	-1.636602	0.944893	-6.621295	Al	-0.950981	-1.647005	-6.581757
C	0.000000	0.000000	6.283786	C	0.000000	0.000000	6.234019
C	0.000000	0.000000	-6.283786	C	0.000000	0.000000	-6.234019

B3LYP

$^1S_6$ $K_3(CAl_3)_4$		-4861.724714 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	3.177352
Al	1.923604	0.000216	3.252436
Al	-0.961989	1.665782	3.252436
Al	-0.961615	-1.665998	3.252436
K	0.000000	0.000000	0.000000
Al	0.961989	-1.665782	-3.252436
Al	0.961615	1.665998	-3.252436
Al	-1.923604	-0.000216	-3.252436
K	0.000000	0.000000	6.645457
Al	0.945610	1.637307	9.890026
Al	-1.890754	0.000269	9.890026
Al	0.945144	-1.637575	9.890026
C	0.000000	0.000000	-3.177352
C	0.000000	0.000000	9.550311
K	0.000000	0.000000	-6.645457
C	0.000000	0.000000	-9.550311
Al	1.890754	-0.000269	-9.890026
Al	-0.945610	-1.637307	-9.890026
Al	-0.945144	1.637575	-9.890026

BP86

^1C_i $K_3(CAl_3)_4$		-4861.859513 Hartrees	
Atom	x	y	z
C	0.000391	0.000412	3.149068
Al	0.001305	1.937526	3.227934
Al	-1.677615	-0.967369	3.228417
Al	1.677610	-0.968784	3.228257
K	0.000000	0.000000	0.000000
Al	1.677615	0.967369	-3.228417
Al	-1.677610	0.968784	-3.228257
Al	-0.001305	-1.937526	-3.227934
K	-0.000199	0.000529	6.595023
Al	-1.647585	0.953116	9.823713
Al	-0.000727	-1.902029	9.823892
Al	1.648493	0.951766	9.823419
C	-0.000391	-0.000412	-3.149068
C	0.000033	0.000916	9.476298
K	0.000199	-0.000529	-6.595023
C	-0.000033	-0.000916	-9.476298
Al	0.000727	1.902029	-9.823892
Al	1.647585	-0.953116	-9.823713
Al	-1.648493	-0.951766	-9.823419

B3LYP

$^1D_{3h}$ $K_4(CAl_3)_5$		-6227.129796 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	-0.000000	1.926903	-0.000000
Al	1.668747	-0.963451	-0.000000
Al	-1.668747	-0.963451	-0.000000
K	0.000000	0.000000	3.278985
Al	-1.665843	0.961775	6.502026
Al	1.665843	0.961775	6.502026
Al	-0.000000	-1.923550	6.502026
K	0.000000	0.000000	-3.278985

BP86

$^1C_{3h}$ $K_4(CAl_3)_5$		-6227.307752 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.000000
Al	1.940626	0.000095	0.000000
Al	-0.970231	-1.680679	0.000000
Al	-0.970395	1.680584	0.000000
K	0.000000	0.000000	3.252967
Al	0.968154	1.677678	6.451853
Al	0.968835	-1.677285	6.451853
Al	-1.936988	-0.000393	6.451853
K	0.000000	0.000000	-3.252967

Al	1.665843	0.961775	-6.502026
Al	-0.000000	-1.923550	-6.502026
Al	-1.665843	0.961775	-6.502026
C	0.000000	0.000000	6.406609
C	0.000000	0.000000	-6.406609
K	0.000000	0.000000	9.914551
C	0.000000	0.000000	12.809353
Al	0.000000	1.891254	13.148577
Al	-1.637874	-0.945627	13.148577
Al	1.637874	-0.945627	13.148577
K	0.000000	0.000000	-9.914551
C	0.000000	0.000000	-12.809353
Al	0.000000	1.891254	-13.148577
Al	1.637874	-0.945627	-13.148577
Al	-1.637874	-0.945627	-13.148577

Al	0.968835	-1.677285	-6.451853
Al	-1.936988	-0.000393	-6.451853
Al	0.968154	1.677678	-6.451853
C	0.000000	0.000000	6.351331
C	0.000000	0.000000	-6.351331
K	0.000000	0.000000	9.838169
C	0.000000	0.000000	12.709114
Al	1.903539	-0.000462	13.055718
Al	-0.951370	1.648744	13.055718
Al	-0.952169	-1.648282	13.055718
K	0.000000	0.000000	-9.838169
C	0.000000	0.000000	-12.709114
Al	1.903539	-0.000462	-13.055718
Al	-0.952169	-1.648282	-13.055718
Al	-0.951370	1.648744	-13.055718

B3LYP

$^1C_1$ $K_5(CAl_3)_6$ -7592.533964 Hartrees

Atom	x	y	z
C	-0.017752	0.001286	-0.015067
Al	0.064334	0.005338	1.910643
Al	1.608969	0.004237	-1.049251
Al	-1.725221	0.056237	-0.907641
K	-0.067660	-3.221936	-0.033502
Al	-1.744536	-6.449065	0.981782
Al	1.589614	-6.499266	0.840262
Al	-0.199536	-6.449226	-1.978136
K	0.031325	3.313158	0.013536
Al	1.742924	6.469105	1.062453
Al	0.135128	6.556782	-1.856167
Al	-1.586756	6.546997	0.994442
C	-0.117844	-6.445109	-0.052415
C	0.095911	6.426325	0.064918
K	-0.167752	-9.757078	-0.082086
C	-0.233812	-12.870117	-0.134719
Al	-0.275612	-13.001911	1.786214
Al	-1.879717	-12.911398	-1.134157
Al	1.449392	-12.991210	-1.063233
K	0.186837	9.940533	0.125155
C	0.283466	12.831537	0.188246
Al	0.236900	13.130163	2.085801
Al	1.960116	13.130350	-0.701403
Al	-1.312449	13.245321	-0.798522
K	-0.326260	-16.384406	-0.197077
C	-0.420929	-19.275456	-0.263023

BP86

$^1C_1$ $K_5(CAl_3)_6$ -7592.755077 Hartrees

Atom	x	y	z
C	3.194267	0.006219	-0.004395
Al	3.221866	-1.236597	1.486714
Al	3.219981	-0.663727	-1.826343
Al	3.215045	1.919042	0.326151
K	0.000006	-0.000922	-0.002279
Al	-3.220310	0.662352	1.821320
Al	-3.214910	-1.920723	-0.330812
Al	-3.221630	1.234780	-1.491794
K	6.487030	0.015258	-0.002953
Al	9.670873	-1.899806	-0.314944
Al	9.676164	1.237289	-1.503646
Al	9.673643	0.698566	1.807652
C	-3.194261	-0.007863	-0.000530
C	9.565673	0.012189	-0.003485
K	-6.487016	-0.017358	-0.002631
C	-9.565649	-0.014155	-0.004221
Al	-9.675404	-1.239343	1.495791
Al	-9.670012	1.897949	0.306467
Al	-9.675233	-0.700884	-1.815295
K	13.068862	0.007993	0.004529
C	15.935038	-0.010893	0.006285
Al	16.272432	-1.195964	1.498298
Al	16.277719	-0.713633	-1.763765
Al	16.292923	1.870164	0.284995
K	13.068921	-0.006156	0.001429
C	15.935063	0.014876	0.006633

Al	-0.374485	-19.573166	-2.160754	Al	16.275092	1.199699	-1.484976
Al	1.175528	-19.688112	0.723284	Al	16.295209	-1.865990	-0.270491
Al	-2.097523	-19.576551	0.625942	Al	16.272791	0.718386	1.777330