Electronic Supplementary Material (ESI) for Chemical Communications.

SUPPLEMENTARY INFORMATION

CAl_{11}^-: A molecular rotor with a quasi-planar tetracoordinate carbon

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MOVIE

The short movies extracted from the BOMD simulations for the global minimum structure of CAl_{11}^-. The simulations were performed at 500 K for over 30 ps; and the movies roughly cover a time span of 8 ps.

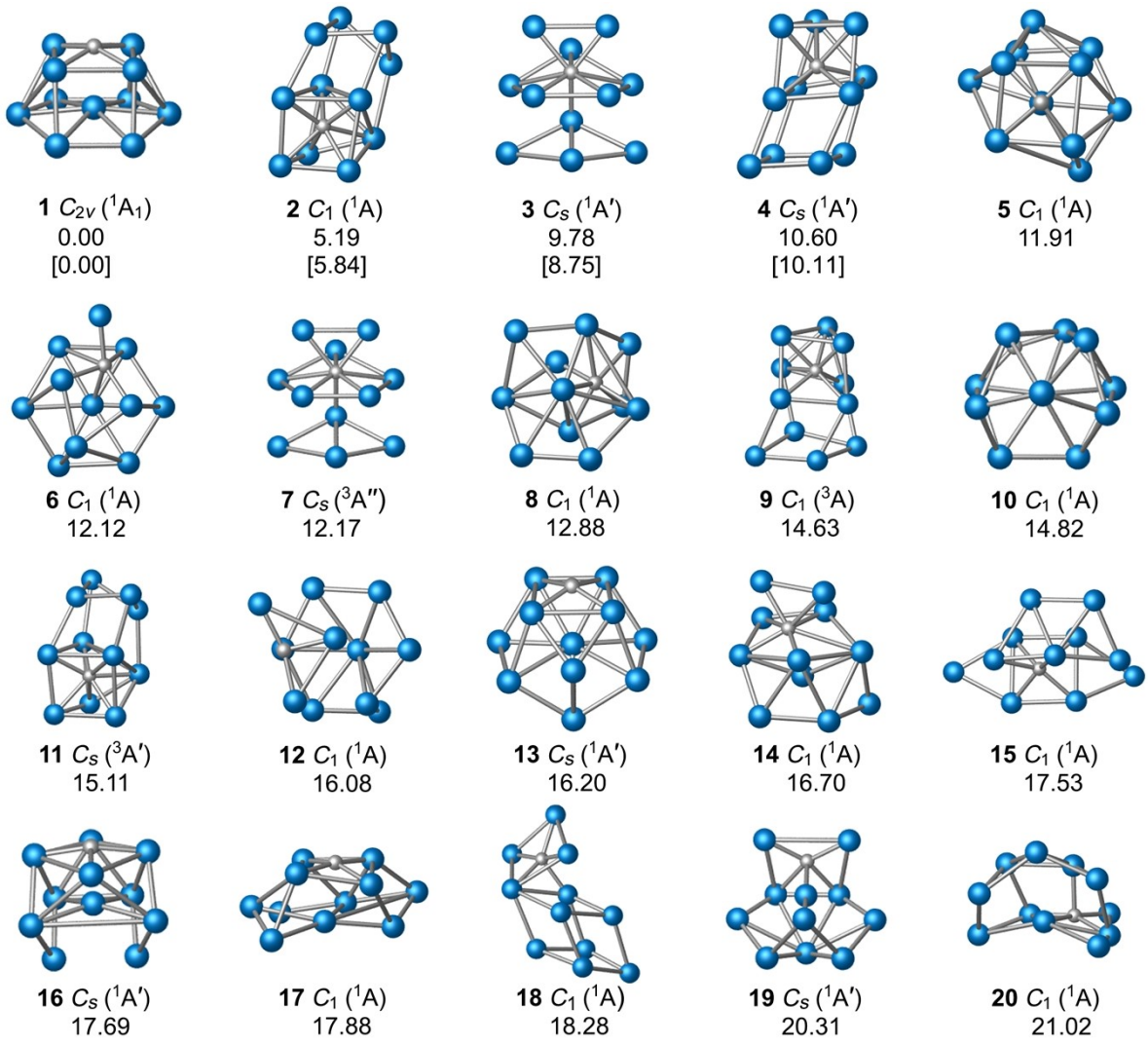

Figure S1. PBE0/def2-QZVP structures for the 20 lowest-energy isomers of CAl_{11}^-. The relative energies are computed at the PBE0/def2-QZVP level, including the ZPE computed at the same level. The single point energies of the first four isomers were recomputed at CCSD(T)/def2-QZVP//PBE0/def2-QZVP (in square brackets). Energies are in kcal mol^{-1}.

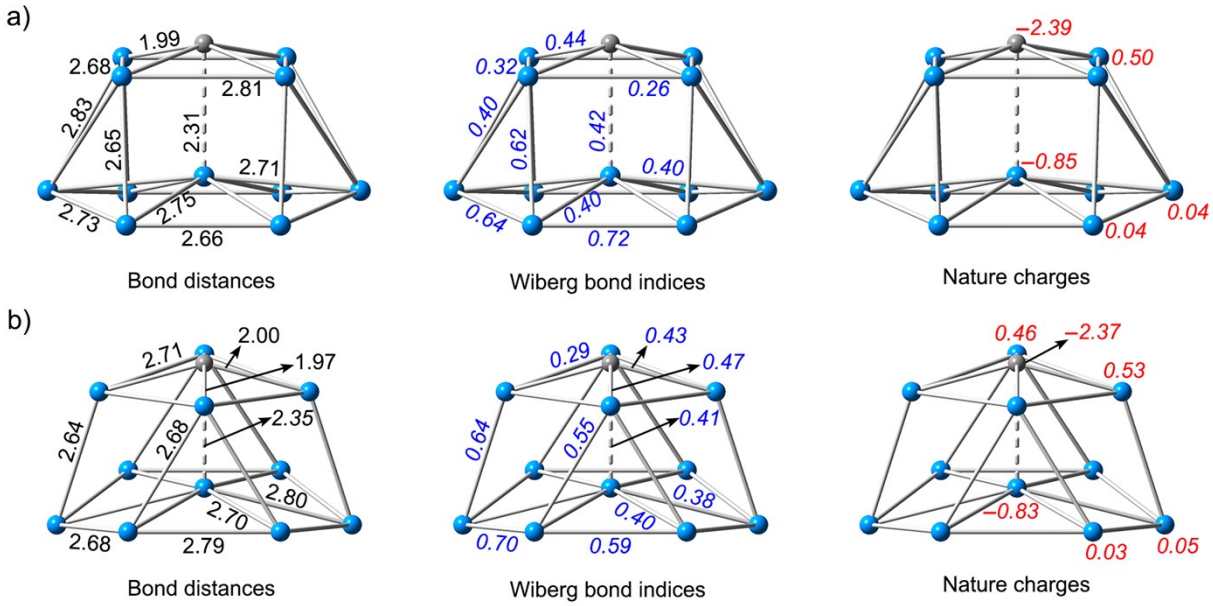

Figure S2. Computed bond lengths (in Å; black color), Wiberg bond indices (blue color), and natural atomic charges (in |e|; red color) for **1** and **TS** structures.

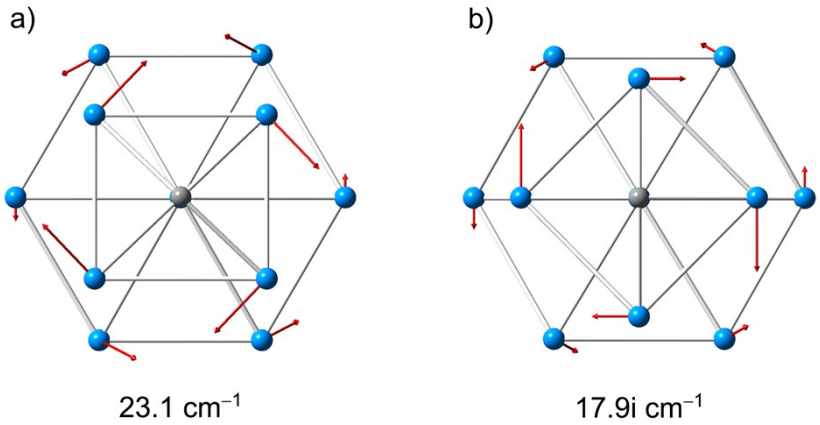

Figure S3. The lowest vibrational frequency of 1 and TS computed at the PBE0/def2-QZVP level.

Cartesian coordinates at the PBE0/def2-QZVP level of structure 1 and the transition state TS

1 (C_{2v}, $^1A_1$)

C	0.00000000	0.00000000	-1.79357100
Al	-1.33946100	1.40617000	-1.37889900
Al	-1.33946100	-1.40617000	-1.37889900
Al	1.33946100	-1.40617000	-1.37889900
Al	1.33946100	1.40617000	-1.37889900
Al	-2.34019700	1.33195900	1.07776100
Al	-2.34019700	-1.33195900	1.07776100
Al	0.00000000	-2.69840500	0.75949500
Al	2.34019700	-1.33195900	1.07776100
Al	2.34019700	1.33195900	1.07776100
Al	0.00000000	2.69840500	0.75949500
Al	0.00000000	0.00000000	0.51336300

TS (C_{2v}, $^1A_1$)

C	0.00000000	0.00000000	-1.80017700
Al	0.00000000	1.92234800	-1.25781000
Al	-2.20698600	1.54338100	0.77378900
Al	-1.93717500	0.03680400	-1.47260300
Al	0.18000300	2.70245600	1.25339100
Al	1.93717500	-0.03680400	-1.47260300
Al	0.00000000	-1.92234800	-1.25781000
Al	2.38536200	1.24487800	0.84178900
Al	0.00000000	0.00000000	0.55373800
Al	-0.18000300	-2.70245600	1.25339100
Al	2.20698600	-1.54338100	0.77378900
Al	-2.38536200	-1.24487800	0.84178900