Supporting Information: Density Functional Description of Alkalides: Introducing the Alkalide State

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TABLE I: List of the alkalide crystals for which calculations were conducted in this work and the. QTAIM charges for the alkali cations and anions, and atomic volumes for the alkali anions (in atomic units), are also given. No atomic relaxation is permitted.

CSD Code	Formula	Alkali Charge	Alkalide Charge	Alkalide Volume
REGCIP	$Rb^+(18C6)(CH_3NH_2)Na^-$	0.857	-0.417	645.0
FABMEA10	$Rb^+(15C5)_2Na^-$	0.888	-0.462	745.8
ROGDEW	$Li^+(C211)Na^-$	0.892	-0.478	711.2
COJDIO	$Li^+(18C6)(CH_3NH_2)_2Na^-$	0.888	-0.388	662.5
REGCAH	$K^+(12C4)_2Na^-$	0.872	-0.472	734.2
FABMAW10	$Cs^+(18C6)_2Na^-$	0.917	-0.432	709.1
JEPMEW	$Cs^+(15C5)_2K^-$	0.898	-0.413	1081.7
JAPVEB	$K^+(C222)K^-$	0.866	-0.392	945.8
JEPMIA	$Rb^+(15C5)_2Rb^-$	0.889	-0.264	1000.9
JAPVOL	$Rb^+(18C6)Rb^-$	0.786	-0.396	987.5
JAPVIF	$Rb^+(C222)Rb^-$	0.862	-0.365	1005.7
FUJDAP	$Cs^+(C222)Cs^-$	0.865	-0.360	1225.5
REJBAK	$Li^+(C211)Cs^-$	0.891	-0.220	1052.7