

Table S1. The NEC of the ground state B_nRb_2 ($n=1-12$) clusters

Clusters	NEC		
	Rb-1	Rb-2	B
B_1Rb_2	$5S^{0.38}4d^{0.04}5p^{0.13}$	$5S^{0.38}4d^{0.04}5p^{0.13}$	$2S^{1.90}2p^{2.02}$
B_2Rb_2	$5S^{0.06}4d^{0.04}5p^{0.06}$	$5S^{0.06}4d^{0.04}5p^{0.06}$	$2S^{1.42}2p^{2.42}3p^{0.02}$
B_3Rb_2	$5S^{0.11}4d^{0.02}5p^{0.04}$	$5S^{0.11}4d^{0.02}5p^{0.04}$	$2S^{1.11-1.25}2p^{2.30-2.40}3S^{0.01}3p^{0.01}3d^{0.01-0.02}$
B_4Rb_2	$5S^{0.07}4d^{0.02}5p^{0.02}$	$5S^{0.07}4d^{0.02}5p^{0.02}$	$2S^{0.96-1.08}2p^{2.15-2.66}3S^{0.01}3p^{0.01-0.02}3d^{0.01}$
B_5Rb_2	$5S^{0.06}4d^{0.02}5p^{0.03}$	$5S^{0.04}4d^{0.03}5p^{0.04}5d^{0.01}$	$2S^{0.81-1.20}2p^{1.96-2.77}3S^{0.01}3p^{0.01-0.02}3d^{0.01}$
B_6Rb_2	$5S^{0.02}4d^{0.01}5p^{0.04}$	$5S^{0.02}4d^{0.01}5p^{0.04}$	$2S^{0.86-0.95}2p^{2.38-2.41}3p^{0.01}3d^{0.01}$
B_7Rb_2	$5S^{0.01}4d^{0.02}5p^{0.03}5d^{0.01}$	$5S^{0.01}4d^{0.02}5p^{0.04}5d^{0.01}$	$2S^{0.51-0.86}2p^{2.28-2.90}3p^{0.01-0.06}3d^{0.01}$
B_8Rb_2	$5S^{0.01}5p^{0.03}5d^{0.01}6d^{0.01}$	$5S^{0.01}5p^{0.03}5d^{0.01}6d^{0.01}$	$2S^{0.49-0.83}2p^{2.35-2.43}3p^{0.01-0.08}3d^{0.01}$
B_9Rb_2	$5S^{0.01}4d^{0.02}5p^{0.02}5d^{0.01}$	$5S^{0.01}4d^{0.02}5p^{0.02}5d^{0.01}$	$2S^{0.53-0.86}2p^{2.18-2.59}3S^{0.01}3p^{0.01-0.05}3d^{0.01}$
$B_{10}Rb_2$	$5S^{0.02}4d^{0.04}5p^{0.03}5d^{0.01}6d^{0.01}$	$5S^{0.01}5p^{0.02}5d^{0.02}$	$2S^{0.51-0.86}2p^{2.14-2.72}3p^{0.01-0.02}3d^{0.01}$
$B_{11}Rb_2$	$5S^{0.01}4d^{0.03}5p^{0.02}5d^{0.01}$	$5S^{0.01}4d^{0.03}5p^{0.02}5d^{0.01}$	$2S^{0.51-0.84}2p^{2.24-2.58}3p^{0.01-0.03}3d^{0.01}$
$B_{12}Rb_2$	$5S^{0.02}4d^{0.03}5p^{0.03}6d^{0.01}$	$5S^{0.01}5p^{0.02}5d^{0.02}6d^{0.01}$	$2S^{0.50-0.85}2p^{2.23-2.67}3p^{0.01-0.02}3d^{0.01}$

Table S2. The NEC of the ground state $B_n^-Rb_2$ ($n=1-12$) clusters

Clusters	NEC		
	Rb-1	Rb-2	B
$B_1^-Rb_2$	$5S^{0.77}4d^{0.01}5p^{0.18}$	$5S^{0.77}4d^{0.01}5p^{0.18}$	$2S^{1.93}2p^{2.18}$
$B_2^-Rb_2$	$5S^{0.64}4d^{0.02}5p^{0.11}5d^{0.01}$	$5S^{0.64}4d^{0.02}5p^{0.11}5d^{0.01}$	$2S^{1.44}2p^{2.28}3p^{0.02}$
$B_3^-Rb_2$	$5S^{0.18}5p^{0.16}5d^{0.03}6d^{0.01}$	$5S^{0.18}5p^{0.16}5d^{0.03}6d^{0.01}$	$2S^{1.02-1.25}2p^{2.54-2.59}3p^{0.01}3d^{0.02}4p^{0.01}$
$B_4^-Rb_2$	$5S^{0.40}4d^{0.02}5p^{0.16}6S^{0.01}$	$5S^{0.40}4d^{0.02}5p^{0.16}6S^{0.01}$	$2S^{0.95-1.08}2p^{2.19-2.64}3S^{0.01}3p^{0.01-0.02}3d^{0.01}$
$B_5^-Rb_2$	$5S^{0.45}4d^{0.05}5p^{0.23}$	$5S^{0.22}4d^{0.05}5p^{0.18}5p^{0.01}$	$2S^{0.84-0.95}2p^{2.27-2.78}3S^{0.01}3p^{0.01-0.02}3d^{0.01}4p^{0.01}$
$B_6^-Rb_2$	$5S^{0.11}4d^{0.05}5p^{0.02}5d^{0.01}$	$5S^{0.60}4d^{0.03}5p^{0.23}5d^{0.01}$	$2S^{0.77-0.93}2p^{2.24-2.53}3S^{0.01}3p^{0.01}3d^{0.01}$
$B_7^-Rb_2$	$5S^{0.01}5p^{0.06}5d^{0.01}6d^{0.03}$	$5S^{0.01}5p^{0.06}5d^{0.01}6d^{0.03}$	$2S^{0.55-0.81}2p^{2.56-2.79}3d^{0.01}4p^{0.01-0.07}$
$B_8^-Rb_2$	$5S^{0.68}4d^{0.04}5p^{0.30}5d^{0.01}$	$5S^{0.01}4d^{0.02}5p^{0.04}5d^{0.01}$	$2S^{0.55-0.83}2p^{2.32-2.43}3p^{0.01-0.08}3d^{0.01}$
$B_9^-Rb_2$	$5S^{0.03}4d^{0.03}5p^{0.02}6p^{0.01}6d^{0.01}$	$5S^{0.03}4d^{0.03}5p^{0.02}6p^{0.01}6d^{0.01}$	$2S^{0.58-1.06}2p^{2.22-2.70}3S^{0.01}3p^{0.01-0.04}3d^{0.01-0.02}4p^{0.01}$
$B_{10}^-Rb_2$	$5S^{0.53}4d^{0.03}5p^{0.21}$	$5S^{0.16}4d^{0.10}5p^{0.15}5d^{0.01}$	$2S^{0.54-0.85}2p^{2.16-2.64}3p^{0.01-0.02}3d^{0.01}$
$B_{11}^-Rb_2$	$5S^{0.02}4d^{0.05}5p^{0.03}5d^{0.01}$	$5S^{0.02}4d^{0.05}5p^{0.03}5d^{0.01}$	$2S^{0.54-0.83}2p^{2.35-2.59}3p^{0.01-0.03}3d^{0.01}$
$B_{12}^-Rb_2$	$5S^{0.02}4d^{0.05}5p^{0.04}5d^{0.01}$	$5S^{0.02}4d^{0.05}5p^{0.04}5d^{0.01}$	$2S^{0.64-0.87}2p^{2.23-2.52}3p^{0.01-0.03}3d^{0.01}$