Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Noble Gas Encapsulated B_{40} Cage

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Supporting Information

Table S1. The rate constants (k, Sec^{-1}) for the dissociation process, $Ng@B_{40} \rightarrow Ng + B_{40}$ and $Ng_2@B_{40} \rightarrow Ng + Ng@B_{40}$ computed at the ωB97XD/def2-TZVP//ωB97XD/def2-SVP level.

System	B_7-hole	B_6-hole
	K	k
$He@B_{40}$	$4.7x10^{-50}$	$3.9x10^{-50}$
$Ne@B_{40}$	$1.5x10^{-88}$	$2.6x10^{-89}$
$Ar@B_{40}$	$3.8x10^{-139}$	$4.5x10^{-138}$
$Kr@B_{40}$	$6.0x10^{-111}$	$5.1x10^{-144}$
$Xe@B_{40}$	$5.2x10^{-101}$	$1.9x10^{-133}$
$Rn@B_{40}$	$2.7x10^{-90}$	$7.6x10^{-119}$
$He_2@B_{40}$	$4.0x10^{-31}$	
$Ne_2@B_{40}$	$2.0x10^{-37}$	
$Ar_2@B_{40}$	$7.5x10^{0}$	

Table S2. Ng-Ng interatomic distances in Å unit in free Ng_2 dimer.

System	r(Ng-Ng) in $Ng_2@B_{40}$	r(Ng-Ng) in free Ng_2	$\Delta(r$(Ng-Ng))
$He_2@B_{40}$	1.672	3.174	1.502
$Ne_2@B_{40}$	1.906	3.334	1.428
$Ar_2@B_{40}$	2.232	4.092	1.860
$Kr_2@B_{40}$	2.335	4.308	1.973

Table S3. Electron density descriptors (au) at the bond critical points (BCPs) between two Ng atoms in free Ng_2 dimer.

System	BCP	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$
He_2	He-He	0.0005	0.0032	0.0002
Ne_2	Ne-Ne	0.0011	0.0066	0.0004
Ar_2	Ar-Ar	0.0015	0.0056	0.0004
Kr_2	Kr-Kr	0.0018	0.0064	0.0005

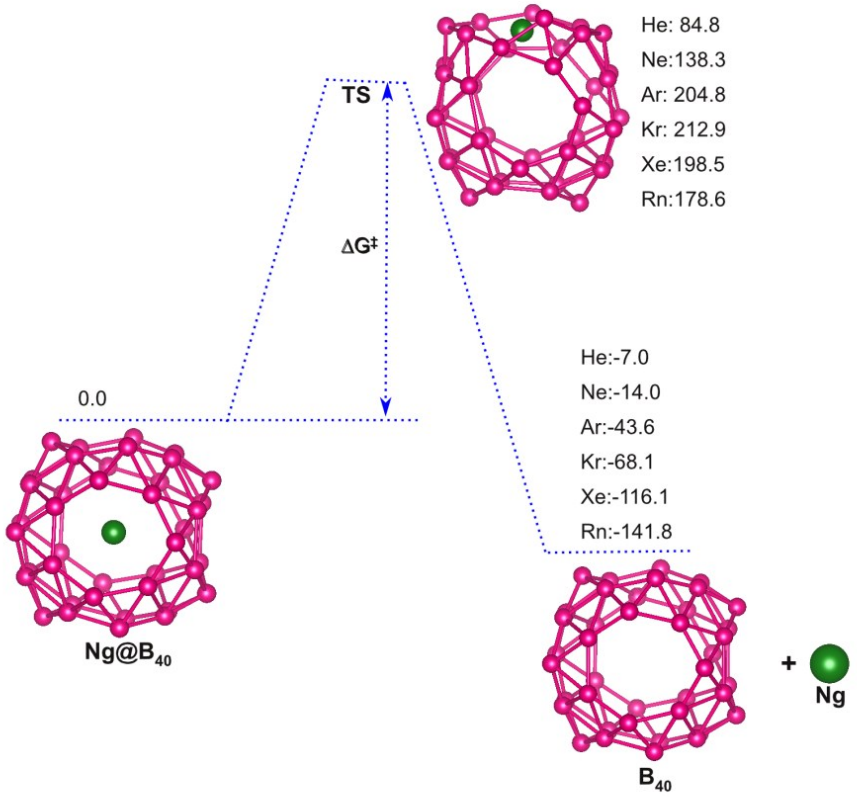

Fig. S1 Activation free energy barrier, $\Delta G^{\ddagger}$, for release of Ng along B_6 hole for $Ng@B_{40}$. $\Delta G^{\ddagger}$ is computed at the ωB97X-D/def2-TZVP//ωB97X-D/def2-SVP level with thermal correction taken from the latter level.

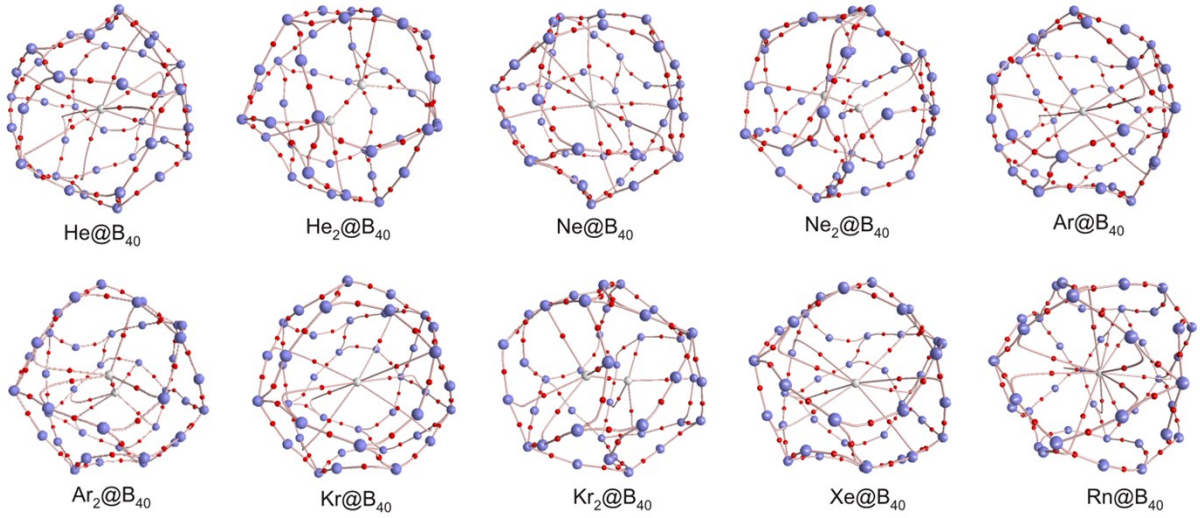

Fig. S2 The molecular graphs of $Ng@B_{40}$ and $Ng_2@B_{40}$ systems showing BCPs.

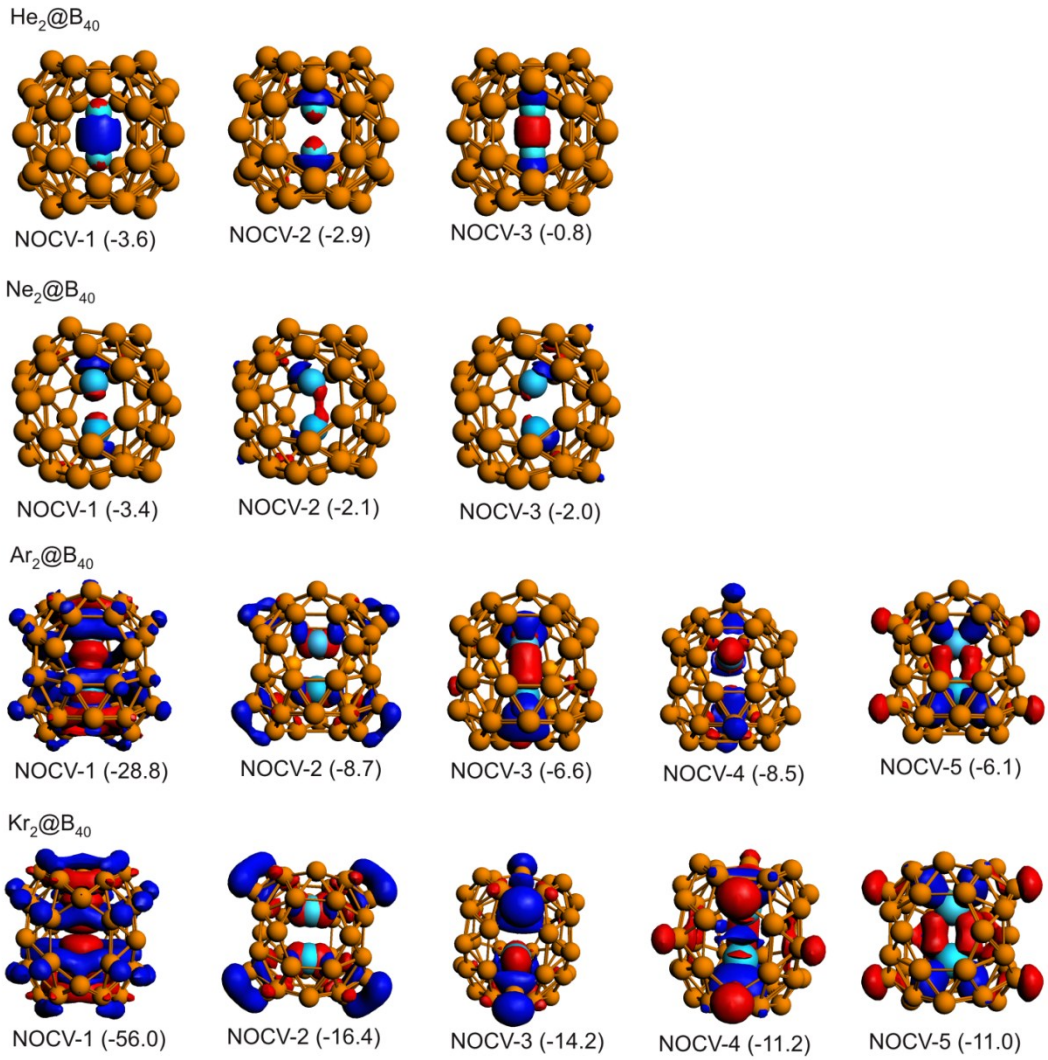

Fig. S3 The difference density plots of the major contributing NOCV orbitals of $Ng_2@B_{40}$ systems. The associated ΔE_{orb} values in kcal/mol are given within parentheses.