Supporting Information for:

Theoretical Study on the Noble-Gas Exchange Reactions of $Ng + HNBNg'^{+} \rightarrow Ng' + HNBNg^{+}$ (Ng, Ng' = He, Ne, Ar, Kr, and Xe)

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Table S1. Calculated reaction energies (in kcal/mol) of the $Ng + HNBNg'^{+} \rightarrow Ng' + HNBNg^{+}$ reactions. (Ng' = He)

(Ng', Ng)	(He,Ne)	(He,Ar)	(He,Kr)	(He,Xe)
MP2/aptz	-0.3	-36.6	-49.7	-64.5
CCSD(T)/aptz//MP2/aptz	-0.3	-36.4	-49.4	-64.4
CCSD(T)/apqz//MP2/aptz	-0.5	-35.6	-48.1	-63.1
CCSD(T)/aptz	-0.3	-34.4	-49.4	-64.4
CCSD(T)/apqz//CCSD(T)/aptz	-0.5	-34.3	-48.1	-63.0

Table S2. Calculated reaction energies (in kcal/mol) of the $Ng + HNBNg'^{+} \rightarrow Ng' + HNBNg^{+}$ reactions. (Ng' = Ne)

(Ng', Ng)	(Ne,Ar)	(Ne,Kr)	(Ne,Xe)
MP2/aptz	-37.0	-50.0	-64.8
CCSD(T)/aptz//MP2/aptz	-36.7	-49.7	-64.7
CCSD(T)/apqz//MP2/aptz	-36.2	-48.7	-63.6
CCSD(T)/aptz	-34.7	-49.8	-64.7
CCSD(T)/apqz//CCSD(T)/aptz	-34.8	-48.6	-63.6

Table S3. Calculated reaction energies (in kcal/mol) of the $Ng + HNBNg'^{+} \rightarrow Ng' + HNBNg^{+}$ reactions. (Ng' = Ar, Kr)

(Ng', Ng)	(Ar,Kr)	(Ar,Xe)	(Kr,Xe)
MP2/aptz	-13.1	-27.8	-14.8
CCSD(T)/aptz//MP2/aptz	-13.0	-28.0	-14.9
CCSD(T)/apqz//MP2/aptz	-12.5	-27.4	-15.0
CCSD(T)/aptz	-15.1	-30.0	-14.9
CCSD(T)/apqz//CCSD(T)/aptz	-13.8	-28.7	-14.9

Table S4. Calculated vibrational frequencies (in cm^{-1}) of Ng–B stretching mode at the MP2/aptz level.

Ng	FNgBO	FNgBNH	$FNgBN^-$	$HNBNg^+$
He	1145 (1.247)[a]	1275 (1.199)	1248 (1.196)	1122 (1.228)
Ne	nc[b]	nc[b]	489 (1.559)	578 (1.504)
Ar	404 (1.802)	409 (1.775)	491 (1.808)	545 (1.765)
Kr	387 (1.953)	413 (1.937)	425 (1.946)	480 (1.897)
Xe	375 (2.155)	393 (2.131)	387 (2.139)	444 (2.073)

[a]The values in parentheses are the predicted Ng–B bond lengths in angstrom.

[b]not calculated (not energy minimum)

Table S5. Calculated rate constants (in cm^3 $molecule^{-1}$ s^{-1}) of the $He + HNBHe^+$ reaction and its three isotopic analogs.

	$He + HNBHe^+$		$^3He + HNBHe^+$		$He + HNB^3He^+$		$^3He + HNB^3He^+$	
T(K)	TST	CVT/SCT	TST	CVT/SCT	TST	CVT/SCT	TST	CVT/SCT
50	1.86(−51)[a]	1.82(−33)	5.14(−52)	2.88(−33)	5.98(−51)	5.46(−32)	1.67(−51)	1.24(−31)
100	1.99(−31)	1.41(−28)	1.17(−31)	1.94(−28)	3.58(−31)	6.86(−28)	2.12(−31)	1.11(−27)
150	9.04(−25)	5.60(−24)	6.83(−25)	5.50(−24)	1.35(−24)	1.12(−23)	1.02(−24)	1.18(−23)
200	1.91(−21)	4.61(−21)	1.63(−21)	4.40(−21)	2.60(−21)	7.13(−21)	2.21(−21)	6.97(−21)
250	1.92(−19)	3.26(−19)	1.74(−19)	3.15(−19)	2.46(−19)	4.49(−19)	2.23(−19)	4.42(−19)
300	4.23(−18)	6.03(−18)	3.98(−18)	5.93(−18)	5.20(−18)	7.78(−18)	4.90(−18)	7.75(−18)
400	2.12(−16)	2.57(−16)	2.08(−16)	2.58(−16)	2.47(−16)	3.07(−16)	2.43(−16)	3.12(−16)
500	2.33(−15)	2.63(−15)	2.34(−15)	2.68(−15)	2.64(−15)	3.02(−15)	2.66(−15)	3.10(−15)
600	1.19(−14)	1.30(−14)	1.22(−14)	1.33(−14)	1.33(−14)	1.45(−14)	1.35(−14)	1.50(−14)

[a] 1.86 (–51) means 1.86×10^{-51}

Table S6. Calculated harmonic and anharmonic zero-point energies (in kcal/mol) of the reactants and transition states of the noble-gas identity exchange reactions at the MP2/aptz level.

	Reactant	Transition state	$\Delta ZPE^{\neq a}$
$He + HNBHe^+$ (R1)	12.41 (12.22)[b]	12.72 (12.50)	0.31 (0.28)
$Ne + HNBNe^+$ (R2)	11.45 (11.29)	11.57 (11.39)	0.12 (0.10)
$Ar + HNBAr^+$ (R4)	11.47 (11.30)	11.36 (11.21)	-0.11 (-0.09)
$Kr+ HNBKr^+$ (R5)	11.37 (11.24)	11.10 (10.96)	-0.27 (-0.28)
$Ar+ HNBAr^+$ (R6)	11.28 (11.15)	10.86 (10.72)	-0.42 (-0.43)

[a] $\Delta ZPE^{\neq}$ = ZPE(transition state) – ZPE(reactant)

[b] The values in parentheses are the anharmonic values.

Table S7. Calculated ratios of the TS anharmonic and harmonic vibrational partition functions of the noble-gas identity exchange reactions.

	$Q_{anh}^{\neq} / Q_{har}^{\neq}$				
Temperature (K)	He	Ne	Ar	Kr	Xe
50.0	1.0001	1.0007	1.0005	1.0018	1.0014
100.0	1.0051	1.0129	1.0061	1.0070	1.0017
150.0	1.0177	1.0330	1.0138	1.0104	0.9977
200.0	1.0346	1.0536	1.0214	1.0125	0.9928
250.0	1.0526	1.0725	1.0283	1.0142	0.9885
300.0	1.0702	1.0892	1.0343	1.0157	0.9851
400.0	1.1016	1.1165	1.0442	1.0183	0.9805
500.0	1.1274	1.1374	1.0519	1.0207	0.9777
600.0	1.1484	1.1540	1.0581	1.0229	0.9763

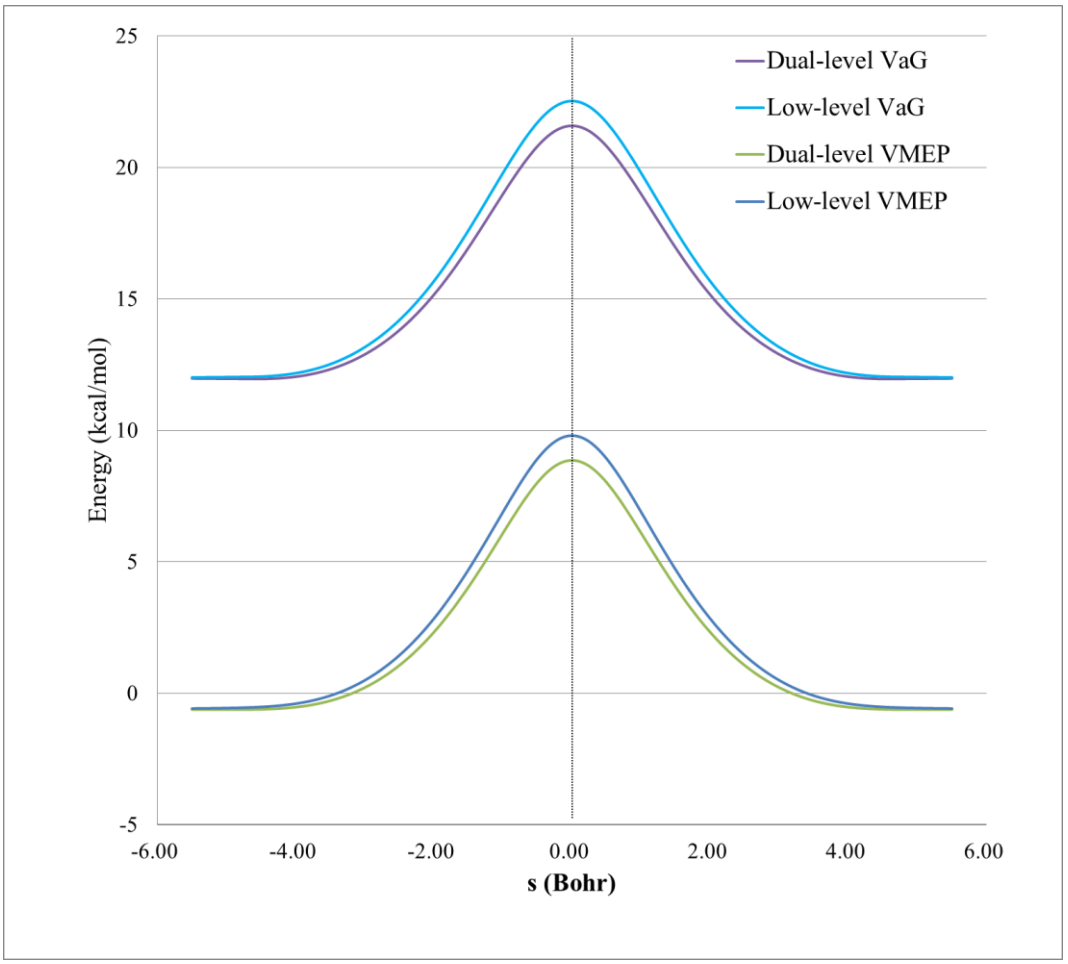

Figure S1. Calculated potential energies along the minimum energy path (V_{MEP}) of the He + HNBHe'$^{+}$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^{G} curves are V_{MEP} plus the vibrational zero point energies along the MEP.

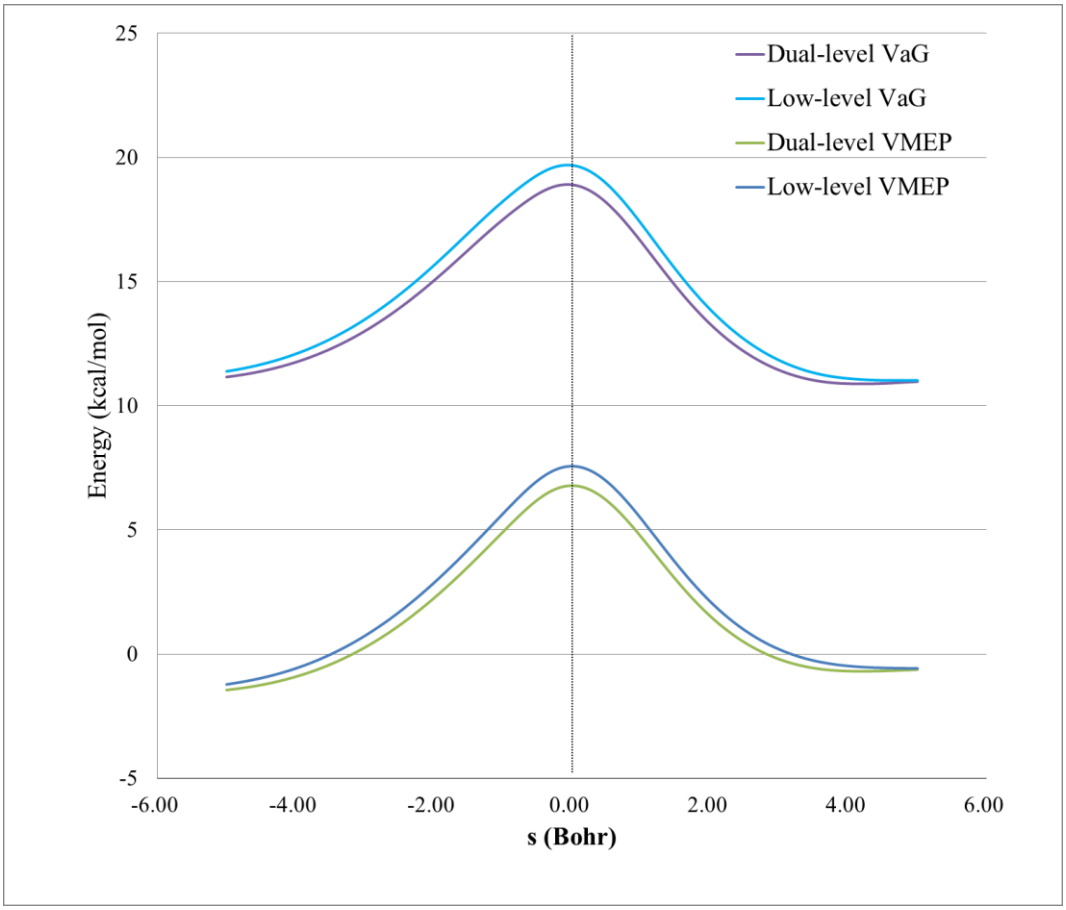

Figure S2. Calculated potential energies along the minimum energy path (V_{MEP}) of the He + $HNBNe^+$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^G curves are V_{MEP} plus the vibrational zero point energies along the MEP.

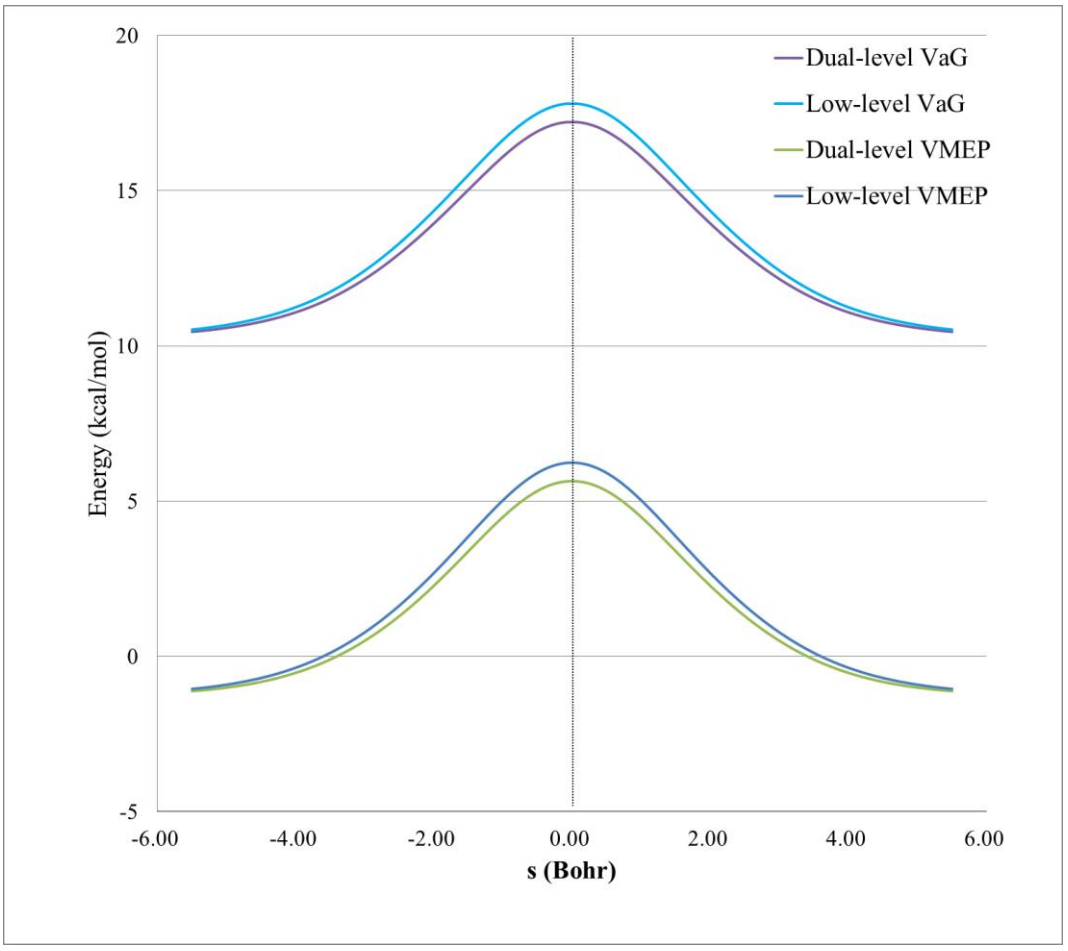

Figure S3. Calculated potential energies along the minimum energy path (V_{MEP}) of the Ne + HNBNe'$^{+}$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^{G} curves are V_{MEP} plus the vibrational zero point energies along the MEP.

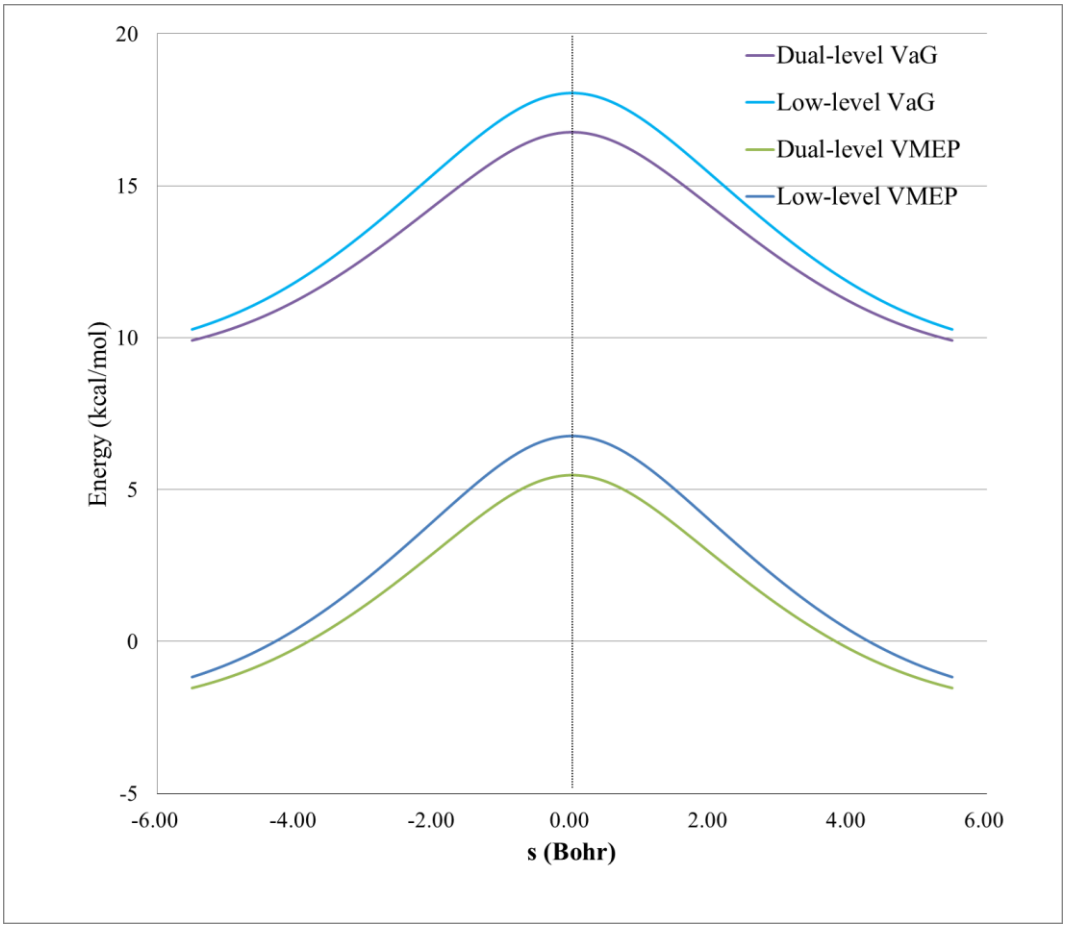

Figure S4. Calculated potential energies along the minimum energy path (V_{MEP}) of the Ar + $HNBAr'^{+}$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^{G} curves are V_{MEP} plus the vibrational zero point energies along the MEP.

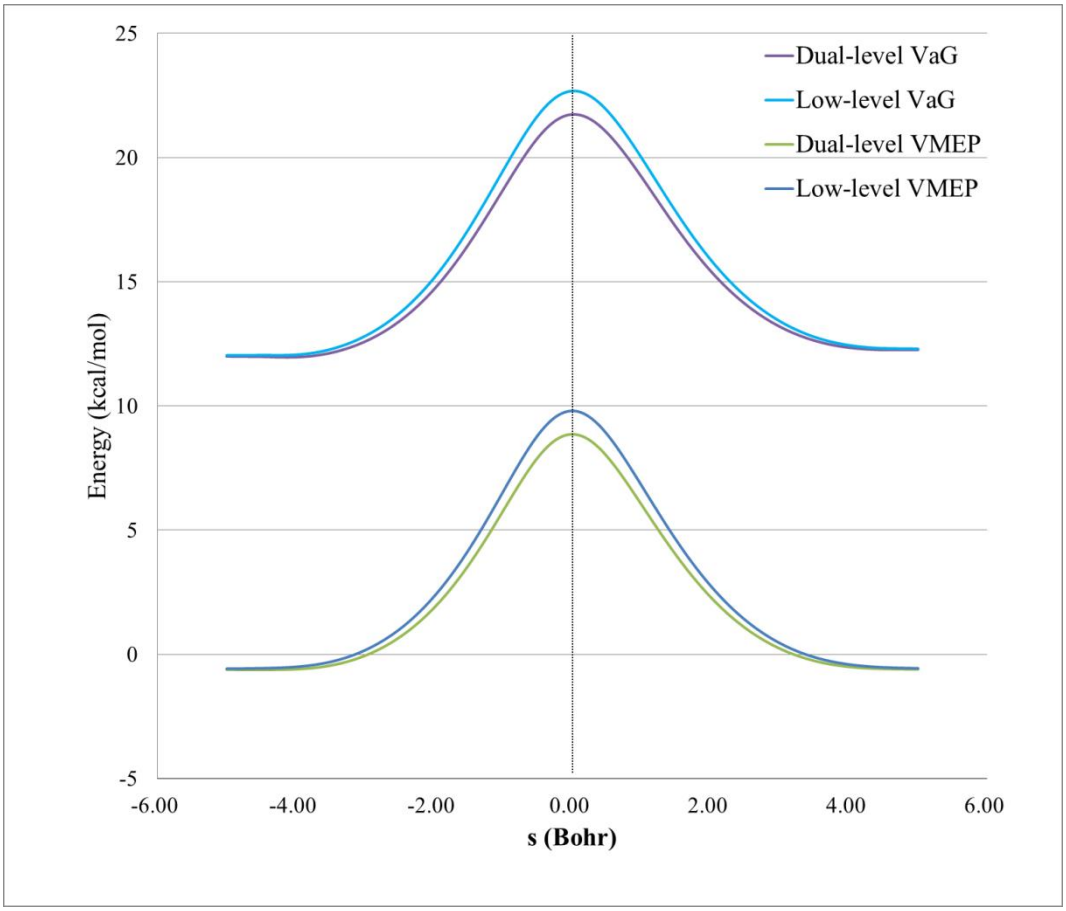

Figure S5. Calculated potential energies along the minimum energy path (V_{MEP}) of the $^{3}He + HNBHe^{+}$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^{G} curves are V_{MEP} plus the vibrational zero point energies along the MEP.

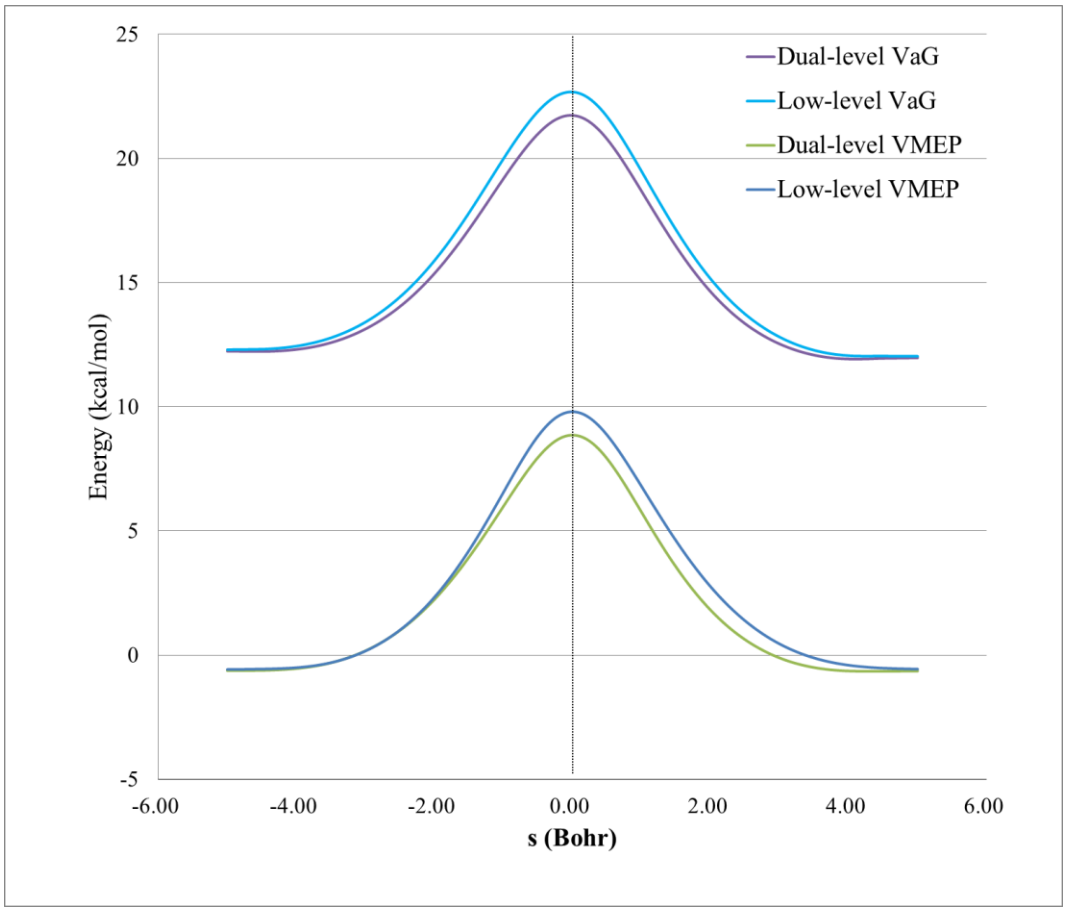

Figure S6. Calculated potential energies along the minimum energy path (V_{MEP}) of the He + HNB^3He^+ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^G curves are V_{MEP} plus the vibrational zero point energies along the MEP.

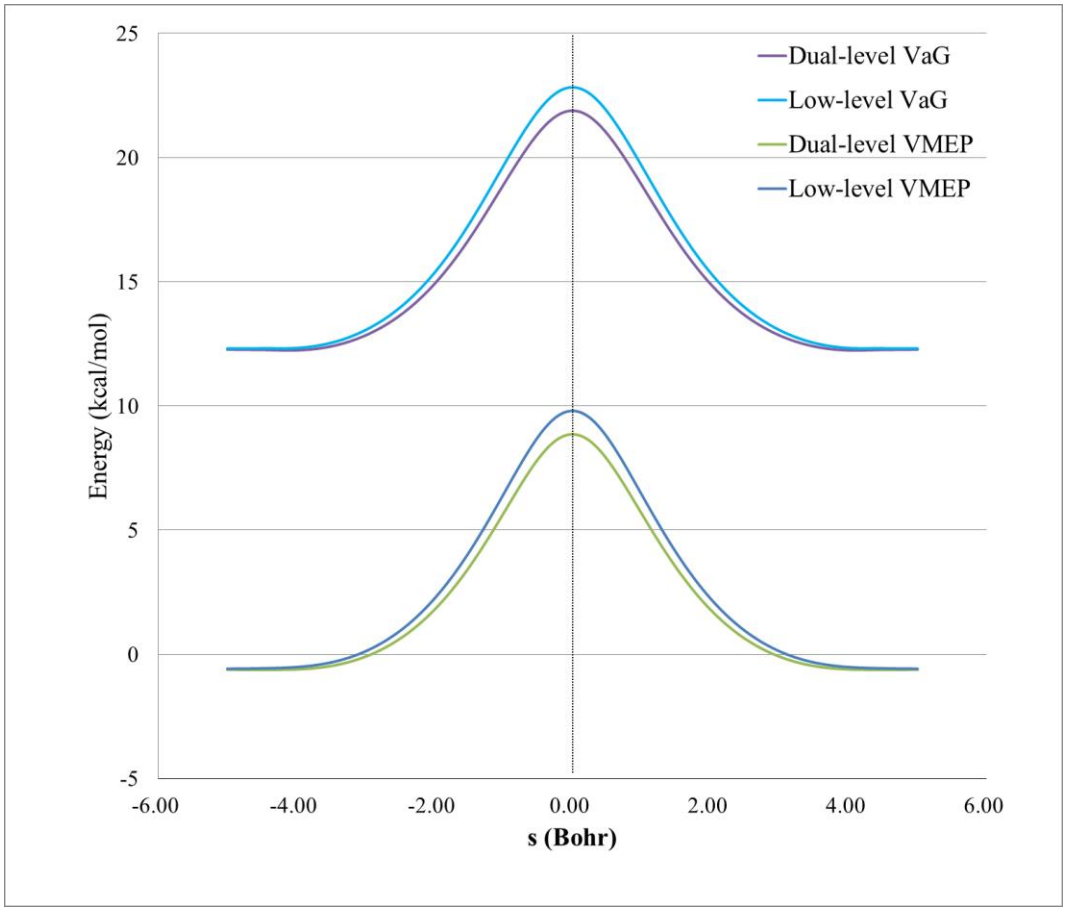

Figure S7. Calculated potential energies along the minimum energy path (V_{MEP}) of the $^{3}He + HNB^{3}He^{+}$ reaction at the MP2/aptz level. The zero of energy is defined as the sum of the energies of the two reactants calculated separately. The Va^{G} curves are V_{MEP} plus the vibrational zero point energies along the MEP.