

Supporting Information

Table 1 – Partitioning of the intergroup exchange energy for the N₂ molecule.

	Scheme I	Scheme II	Sch.II - Sch.I
$\Delta E[x]$ - core/ nb	-	0.3496	-
$\Delta E[x]$ - (core+nb)/ sigma	0.0830	0.1709	0.0879
$\Delta E[x]$ - (core+nb)/ pi	0.0556	0.1053	0.0497
$\Delta E[x]$ - sigma/ pi	-0.0753	-0.1246	-0.0493
$\Delta E[x]$ - pi/ pi	-0.0111	-0.0111	0.0000
$\Delta E[x]$	0.0325	0.4708	0.4383

Table 2 – Partitioning of the reference energy for the N₂ molecule. Intergroup quantities are not shown.

	Scheme I	Scheme II	Sch.II - Sch.I
$\Delta E[\text{ref}]$ - core	-	-9.3478	-
$\Delta E[\text{ref}]$ - nb	-	-4.1446	-
$\Delta E[\text{ref}]$ - sigma	-7.9675	-8.5471	-0.5796
$\Delta E[\text{ref}]$ - pi	-4.6465	-4.6549	-0.0084
$\Delta E[\text{ref}]$ - (core+nb)	-12.6854	-12.3229	0.3625

Table 3 – Partitioning of the reference kinetic energy for the N₂ molecule.

	Scheme I	Scheme II	Sch.II - Sch.I
$\Delta T[\text{ref}]$ - core	-	4.1990	-
$\Delta T[\text{ref}]$ - nb	-	-4.6537	-
$\Delta T[\text{ref}]$ - (core+nb)	-0.4390	-0.4547	-0.0157
$\Delta T[\text{ref}]$ - sigma	1.7887	1.8737	0.0850
$\Delta T[\text{ref}]$ - pi	-0.0091	-0.0013	0.0078
$\Delta T[\text{ref}]$	1.3315	1.4165	0.0850

Table 4 – Partitioning of the reference potential energy for the N₂ molecule.

	Scheme I	Scheme II	Sch.II - Sch.I
$\Delta V[\text{ref}]$ - core	-	-13.5468	-
$\Delta V[\text{ref}]$ - nb	-	0.5091	-
$\Delta V[\text{ref}]$ - sigma	-9.7562	-10.4208	-0.6646
$\Delta V[\text{ref}]$ - pi	-4.6374	-4.6537	-0.0163
$\Delta V[\text{ref}]$ - core/ nb	-	1.1695	-
$\Delta V[\text{ref}]$ - core/ sigma	-	2.9763	-
$\Delta V[\text{ref}]$ - core/ pi	-	1.4621	-
$\Delta V[\text{ref}]$ - nb/ sigma	-	1.0042	-
$\Delta V[\text{ref}]$ - nb/ pi	-	0.8177	-
$\Delta V[\text{ref}]$ - sigma/ pi	1.1058	1.1773	0.0715
$\Delta V[\text{ref}]$ - pi/ pi	0.6874	0.6895	0.0021
$\Delta V[\text{ref}]$ - (core+nb)	-12.2464	-11.8682	0.3782
$\Delta V[\text{ref}]$ - (core+nb)/ sigma	4.0951	4.1458	0.0507
$\Delta V[\text{ref}]$ - (core+nb)/ pi	2.3672	2.2797	-0.0875
$\Delta V[\text{ref}]$	-1.3118	-1.7751	-0.4633