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Richard B. Darzynkiewicz and Gustavo E. Scuseria*: Noble Gas Endohedral Complexes of C_{60} Buckminsterfullerene

Page 7143. The results quoted in Tables 3 and 4 as MP2 are actually Hartree−Fock (HF). The correct MP2 results are listed below (positive energies represent repulsive interactions). All noble gas endohedral complexes of C_{60} are found to be lower in energy (i.e., bound) than the respective reactants. Our results are now in fair agreement with those of Bühl et al. (Bühl, M.; Patchkovskii, S.; Thiel, W. *Chem. Phys. Lett.* **1997**, *275*, 14−18). We thank Walter Thiel for bringing this problem into our attention.

TABLE 3: Binding Energies (kcal/mol)

	$He@C_{60}$	$Ne@C_{60}$	$Ar@C_{60}$	$Kr@C_{60}$	$Xe@C_{60}$
3-21G/MP2// 3-21G/B3LYP	0.0	−0.4	−0.2	4.0	13.2
6-31G**/MP2// 6-31G**/B3LYP	−1.0	−5.2	−6.8	−27.2	

TABLE 4: BSSE Corrected Binding Energies (kcal/mol)

	$He@C_{60}$	$Ne@C_{60}$	$Ar@C_{60}$	$Kr@C_{60}$	$Xe@C_{60}$
3-21G/MP2// 3-21G/B3LYP	0.7	1.4	6.9	15.9	30.3
6-31G**/MP2// 6-31G**/B3LYP[c]	−0.3	−1.9	−2.4	−10.1	

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