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Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes $Ng@C_{60}$ and $Ng_2@C_{60}$ (Ng = He–Xe)

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In the final production stages of this Full Paper an error occurred and as a result of this Tables 2, 3, and 4 were printed incorrectly. The correct versions of the Tables are reproduced below. The editorial office apologizes for this mistake.

Table 2. Reaction energies ΔE_R [kcal mol^{-1}] and lengths [Å] of the C–C bonds at which the reaction took place (R_{full}) and for the bonds formed in the final products (R_{CC}).[a,b]

Bond	Bond type		$He_2@C_{60}$			$Ne_2@C_{60}$			$Ar_2@C_{60}$			$Kr_2@C_{60}$			$Xe_2@C_{60}$		
			ΔE_R	R_{full}	R_{CC}	ΔE_R	R_{full}	R_{CC}	ΔE_R	R_{full}	R_{CC}	ΔE_R	R_{full}	R_{CC}	ΔE_R	R_{full}	R_{CC}
1	A	[6,6]	**−20.9**	1.610	1.572	**−23.1**	1.616	1.574	**−32.2**	1.644	1.567	**−39.9**	1.660	1.563	**−44.9**	1.676	1.554/1.561
2	A	[6,6]	**−20.4**	1.605	1.575	**−23.1**	1.616	1.574	**−32.1**	1.644	1.567	**−39.9**	1.660	1.563	−43.3	1.680	1.559
3	A	[6,6]	**−20.4**	1.608	1.575	**−21.1**	1.614	1.575	−21.4	1.636	1.575	−22.4	1.650	1.575	−22.3	1.645	1.574/1.576
a	D	[5,6]	−4.4	1.636	1.572	−6.4	1.641	1.572	−15.3	1.661	1.567	−24.1	1.671	1.560	**−44.6**	1.682	1.552
b	D	[5,6]	−4.2	1.636	1.572	−4.8	1.639	1.572	−15.3	1.661	1.567	−24.1	1.671	1.560	**−44.5**	1.682	1.552
c	D	[5,6]	−5.0	1.638	1.571	−5.0	1.641	1.570	−6.6	1.654	1.570	−7.1	1.664	1.570	−16.6	1.670	1.564/1.567
d	D	[5,6]	−4.2	1.636	1.572	−4.8	1.639	1.572	−6.0	1.652	1.572	−6.5	1.662	1.571	−15.7	1.669	1.568/1.565
e	D	[5,6]	−4.9	1.638	1.571	−5.3	1.641	1.570	−15.9	1.662	1.565	−24.7	1.673	1.558	**−45.5**	1.682	1.550
f	D	[5,6]	−4.9	1.638	1.571	−5.2	1.641	1.570	−2.3	1.613	1.574	−1.3	1.608	1.574	−9.5	1.606	1.571

[a] Reaction energies for free C_{60} are −20.7 and −4.6 kcal mol^{-1} for the [6,6] and [5,6] bonds, respectively. [b] In boldface: bonds that are most reactive under thermodynamic control.

Table 3. Bond lengths R_{CC} [Å] and pyramidalization angles θ_p [°] for the bond types in free and endohedral fullerenes.[a]

Bond	Bond type		$He_2@C_{60}$		$Ne_2@C_{60}$		$Ar_2@C_{60}$		$Kr_2@C_{60}$		$Xe_2@C_{60}$	
			R_{CC}	θ_p[b]	R_{CC}	θ_p[b]	R_{CC}	θ_p[b]	R_{CC}	θ_p[b]	R_{CC}	θ_p[b]
1	A	[6,6]	1.400	11.67	1.403	11.75	1.418	12.08	1.427	12.30	1.432	12.63
2	A	[6,6]	1.398	11.63	1.397	11.60	1.394	11.51	1.395	11.45	1.401	11.16
3	A	[6,6]	1.398	11.62	1.399	11.57	1.403	11.32	1.406	11.14	1.422	11.90
a	D	[5,6]	1.454	11.73	1.459	11.94	1.475	12.63	1.489	12.85	1.502	12.51
b	D	[5,6]	1.454	11.62	1.455	11.58	1.460	11.52	1.466	11.60	1.472	11.95
c	D	[5,6]	1.454	11.63	1.456	11.59	1.462	11.42	1.466	11.30	1.470	11.53
d	D	[5,6]	1.454	11.63	1.456	11.59	1.462	11.42	1.466	11.29	1.470	11.53
e	D	[5,6]	1.454	11.62	1.455	11.59	1.460	11.52	1.466	11.60	1.472	11.96
f	D	[5,6]	1.452	11.62	1.450	11.57	1.443	11.32	1.440	11.14	1.430	11.90

[a] For comparison, the [6,6] and [5,6] distances in free C_{60} at the BP86/TZP level are 1.398 and 1.453 Å, and $\theta_p = 11.64°$. [b] Pyramidalization angles averaged over both atoms that constitute the bond under consideration.

Table 4. Activation energies $\Delta E^{\neq}$ [kcal mol^{-1}] and lengths R_{CC} [Å] of the C–C bonds that will be finally bound.[a,b]

Bond	Bond type		$He_2@C_{60}$		$Ne_2@C_{60}$		$Ar_2@C_{60}$		$Kr_2@C_{60}$		$Xe_2@C_{60}$	
			$\Delta E^{\neq}$	R_{CC}	$\Delta E^{\neq}$	R_{CC}	$\Delta E^{\neq}$	R_{CC}	$\Delta E^{\neq}$	R_{CC}	$\Delta E^{\neq}$	R_{CC}
1	A	[6,6]	**12.8**	2.274/2.250	**11.9**	2.278/2.270	**8.4**	2.366/2.388	**6.2**	2.404/2.403	**4.9**	2.193/2.569
2	A	[6,6]	**13.1**	2.210/2.311	**11.8**	2.290/2.255	**8.5**	2.336/2.336	**6.1**	2.402/2.402	**3.8**	3.065/2.140
3	A	[6,6]	**13.1**	2.268/2.252	**13.0**	2.259/2.265	12.2	2.137/2.419	11.7	2.137/2.426	11.3	2.144/2.411
a	D	[5,6]	21.4	2.595/1.702	20.2	2.623/1.702	15.6	3.049/1.850	12.5	3.315/1.952	5.7	3.511/2.122
b	D	[5,6]	21.5	1.699/2.589	21.3	1.695/2.594	15.7	1.700/2.836	12.6	1.948/3.311	5.6	2.119/3.505
c	D	[5,6]	20.4	1.704/2.578	20.0	1.702/2.581	19.2	1.700/2.595	18.7	1.695/2.600	14.7	1.898/3.152
d	D	[5,6]	21.5	2.590/1.699	21.4	2.591/1.698	20.1	2.605/1.690	19.6	2.598/1.682	8.1	2.052/3.561
e	D	[5,6]	20.4	2.576/1.705	20.0	2.585/1.705	14.9	1.710/2.853	11.9	1.961/3.240	6.1	2.125/3.242
f	D	[5,6]	20.4	2.577/1.705	20.1	2.593/1.703	19.4	2.558/1.693	21.5	2.524/1.696	16.4	3.229/1.893

[a] Activation energies for free C_{60} are 12.7 and 21.0 kcal mol^{-1} for the [6,6] and [5,6] bonds, respectively. [b] In boldface: the bonds that are most reactive under kinetic control.

