

| | G/ C ₆₀ F ₄₈ (Ω) | (G/ C ₆₀ F ₄₈) ₂ (Ω) |
|---------------------------------------|--|--|
| /Start | 127 | 42 |
| 50°C, N ₂ , 15 min | 123 | 41 |
| 100°C, N ₂ , 15 min | 127 | 37 |
| 150°C, N ₂ , 15 min | 112 | 38 |
| 200°C, N ₂ , 15 min | 156 | 48 |
| 22°C, 60%RH air, 3 h | 148 | 47 |
| 22°C, 60%RH air, 20 h | 136 | 49 |
| 150°C, 60%RH air, ^a 15 min | 133 | 46 |
| 150°C, 95%RH air, ^a 15 min | 133 | 48 |
| End | 133 | 48 |

Footnote

^a RH = relative humidity of ambient air (22°C) flowed into chamber. Sample on heated plate.

Supplementary Table 1. Resistance in Ohms of G/ C₆₀F₄₈ and (G/ C₆₀F₄₈)₂ assemblies on 300-nm thick SiO₂/ Si wafers, taken sequentially through different treatments. All resistance measurements were performed in N₂ at 22°C. The robustness of these samples to brief heating in both N₂ and even wet ambient air is evident.

| | Theory | | Experiment |
|-----------------------------------|-----------|-----------|---|
| | 6-311g(d) | 6-31g+(d) | |
| Ionization potential | | | |
| C ₆₀ | 7.65 | 7.64 | 7.61 ±0.06 |
| C ₆₀ F ₁₈ | 9.0 | 9.06 | |
| C ₆₀ F ₃₆ | 11.3 | 11.46 | |
| C ₆₀ F ₄₈ | 12.0 | 12.2 | 12.3 ±0.1{Steger, 1997 #72} |
| F ₄ -TCNQ | 9.24 | 9.32 | |
| 1 st electron affinity | | | |
| C ₆₀ | 2.64 | 2.64 | 2.67 ±0.02 |
| C ₆₀ F ₁₈ | 3.02 | 3.09 | |
| C ₆₀ F ₃₆ | 3.23 | 3.42 | |
| C ₆₀ F ₄₈ | 3.74 | 4.00 | 4.06 ±0.3 (adiabatic){Jin, 1994 #5; Hettich, 1994 #65} |
| F ₄ -TCNQ | 4.47 | 4.56 | |
| 2 nd electron affinity | | | |
| C ₆₀ | <0 | <0 | <0 |
| C ₆₀ F ₁₈ | <0 | 0.08 | |
| C ₆₀ F ₃₆ | 0.61 | 0.86 | |
| C ₆₀ F ₄₈ | 1.82 | 2.13 | |
| F ₄ -TCNQ | 0.12 | 0.33 | |

Supplementary Table 2. Computed values are for vertical transitions. 6-311g(d) is sufficient to predict E_A accurately for C₆₀. Diffuse functions not required. The adiabatic E_A can be evaluated as the mean of the vertical E_A s computed at the ground-state geometry of the initial state and of the final state. For C₆₀, the adiabatic E_A is 0.09 eV larger than the vertical E_A for the initial ground-state geometry. For C₆₀F₄₈, this is ca. 0.2 eV; for C₆₀F₄₈⁻, 0.3 eV; for C₆₀F₃₆, 0.08 eV; for C₆₀F₁₈, 0.14 eV; for F₄-TCNQ, 0.17 eV. The results converge to yield the I_p of C₆₀F₄₈ at 12.1 eV (expt, 12.3±0.1 eV){Steger, 1997 #72}, first adiabatic E_A at 4.0–4.3 eV (expt, 4.06±0.3 eV){Jin, 1994 #5}