Semiconductor-based sensors are widely used for the identification of multi-component chemical and biological mixtures. In recent years, diamond has received a great deal of interest as a potential sensor material due to its mechanical robustness and its property to modify its electrical characteristics according to its surface termination and adsorbed chemical agents. Previous studies have suggested that an adsorbed molecule can localize a free valency in the same way a surface trap can. The present work focuses on molecules chemisorbed to the oxygen-terminated surfaces of high-purity CVD single crystal (100) diamond plates. To investigate the adsorbate-induced surface energy states, an ultra-sensitive, non-steady state interrogation device called Charge-based Deep-Level Transient Spectrometer (Q-DLTS) was built and tested. Potentially, a given adsorbed molecule can be uniquely related to a new surface energy state, thus producing a characteristic spectral signature. This technology is named Quantum Fingerprint. The Q-DLTS system was used to investigate the effect of various monohydric alcohols and benzene derivatives on the surface states of single crystal oxygen-terminated diamond plates. It was found that both types of molecules produce a primary large spectral peak and a smaller, transient one. In the alcohol response, both peaks display a consistent increase in amplitude (i.e., charge output) as the molecule’s carbon content becomes larger. The secondary peak also shows a faster emission rate with higher alcohol molecules. This is attributed to the appearance of new surface states. The secondary peak of the benzene derivative, however, disappears a few minutes after the initial introduction. This is believed to be a physisorption effect.