

### Full CI Carbon Atom and Carbon Cation Energies

	C ( <sup>3</sup> P)			C <sup>+</sup> ( <sup>2</sup> P)		
Basis	E(FCI)	E(CBS(1/( $\ell_{\max}^{3.5}$ ))	E(CBS(1/( $\ell_{\max} + \frac{1}{2}$ ) <sup>4</sup> ))	E(FCI)	E(CBS(1/( $\ell_{\max}^{3.5}$ ))	E(CBS(1/( $\ell_{\max} + \frac{1}{2}$ ) <sup>4</sup> ))
aCV6Z	-37.843854			-37.430004		
aCV7Z	-37.844252	-37.844808	-37.844766	-37.430345	-37.430822	-37.430787
aCV8Z	-37.844356	-37.844531	-37.844517	-37.430413	-37.430526	-37.430516

### Nonrelativistic Full CI Carbon Atom Ionization Potential

Basis	I.P.	E(CBS(1/( $\ell_{\max}^{3.5}$ ))	E(CBS(1/( $\ell_{\max} + \frac{1}{2}$ ) <sup>4</sup> ))	CBS(avg.)
aCV6Z	90829.6 (259.605)			
aCV7Z	90842.1 (259.731)	90,859.4 (259.780)	90,857.9 (259.776)	90,858.7 (259.778)
aCV8Z	90850.0 (259.753)	90,863.6 (259.792)	90,862.7 (259.790)	90,863.2 (259.791)

Values in parentheses are in kcal/mol.

### Relativistic, Nonadiabatic Full CI Carbon Atom Ionization Potential and Errors with Respect to Experiment

Basis	I.P.	E(CBS(1/( $\ell_{\max}^{3.5}$ ))	E(CBS(1/( $\ell_{\max} + \frac{1}{2}$ ) <sup>4</sup> ))	CBS(avg.)
aCV6Z	90798.6 (-21.8)			
aCV7Z	90811.1 (-9.3)	90,828.4 (8.0)	90,826.9 (6.5)	90,827.7 (7.3)
aCV8Z	90819.0 (-1.4)	90,832.6 (12.2)	90,831.7 (11.3)	90,832.2 (11.8)

Errors in parentheses with respect to experiment  $90,820.4 \pm 0.8 \text{ cm}^{-1}$ . The relativistic correction is  $-30.0 \text{ cm}^{-1}$  (X2C). The DBOC correction is  $-0.5 \text{ cm}^{-1}$  and the Breit+QED correction is  $-0.5 \text{ cm}^{-1}$ .