

Instead of doing X2C correction at FCIQMC/aug-cc-pCV7Z level, Table 2 says we can do it at a lower level then add correction

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Table I. Basis set dependence is negligible for (X2C-NR), but correlation dependence is significant.

Hamiltonian	Correlation level	Basis set	$C(^3P)$ E_h	$C(^1D)$ E_h	$E_{1D} - E_{3P}$ E_h	$E_{1D} - E_{3P}$ cm^{-1}
NR,CN	CCSD	aCV4Z-UNC	-37.837 409 963	-37.782 004 291	0.055 405 673	12 160.140
	CCSD	aCV5Z-UNC	-37.839 537 317	-37.784 365 975	0.055 171 342	12 108.710
	CCSD	Extrapolated				
	CCSDT	aCV2Z-UNC	-37.812 913 02	-37.756 420 65	0.056 492 37	12 398.642
	CCSDT	aCV3Z-UNC	-37.833 703 41	-37.781 995 27	0.051 708 14	11 348.625
	CCSDT	aCV4Z-UNC	-37.840 788 965	-37.789 986 684	0.050 802 281	11 149.812
	CCSDT	aCV5Z-UNC	-37.842 966 635	-37.792 478 606	0.050 488 029	11 080.842
	CCSDT	Extrapolated				
	CCSDTQ	aCV2Z-UNC	-37.812 968 91	-37.760 225 59	0.052 743 32	11 575.821
	CCSDTQ	aCV3Z-UNC	-37.833 765 603	-37.785 822 996	0.047 942 607	10 522.186
	CCSDTQ	aCV4Z-UNC	-37.840 855 553	-37.793 812 924	0.047 042 629	10 324.664
	CCSDTQ	aCV5Z-UNC	-37.843 034 101	-37.796 300 155	0.046 733 946	10 256.915
	CCSDTQ	Extrapolated				
	CCSDTQP	aCV2Z-UNC	-37.812 969 17	-37.760 270 44	0.052 698 730	11 566.034
	CCSDTQP	aCV3Z-UNC	running	-37.785 889 727		
	CCSDTQP	aCV4Z-UNC	-37.840 856	running		-
	CCSDTQP	Extrapolated				
	FCI	aCV2Z-UNC	-37.812 969 17	-37.760 270 84	0.052 698 330	11 565.947
	FCI	aCV3Z-UNC	-37.831 626 69	-37.785 890 02		
	FCI	CV4Z-NR	-37.840 156 06			
	FCI	aCV5Z-NR	-37.840 485 35			
	FCIQMC	aCV7Z-NR	-37.844 251 5(08)	-37.797 803(4)		10 194.5(9)
X2C,CN	CCSD	aCV4Z-UNC	-37.852 553 250	-37.797 159 268	0.055 393 982	12 157.574
	CCSD	aCV5Z-UNC	-37.854 697 137	-37.799 537 444	0.055 159 694	12 106.153
	CCSDT	aCV2Z-UNC	-37.827 949 25	-37.771 474 31	0.056 474 94	12 394.817
	CCSDT	aCV3Z-UNC	-37.848 791 52	-37.797 099 12	0.051 692 4	11 345.170
	CCSDT	aCV4Z-UNC	-37.855 930 962	-37.805 144 295	0.050 786 666	11 146.385
	CCSDT	aCV5Z-UNC	-37.858 125 173	-37.807 652 723	0.050 472 450	11 077.422
	CCSDTQ	aCV2Z-UNC	-37.828 005 09	-37.775 276 01	0.052729080	11 572.695
	CCSDTQ	aCV3Z-UNC	-37.848 853 669	-37.800 923 608	0.047 930 062	10 519.433
	CCSDTQ	aCV4Z-UNC	-37.855 997 501	-37.808 967 343	0.047 030 159	10 321.927
	CCSDTQ	aCV5Z-UNC	crashed	crashed		
	CCSDTQP	aCV2Z-UNC	-37.828 005 31	-37.775 320 78	0.05268453	11 562.918
	CCSDTQP	aCV3Z-UNC	running			
	FCI	aCV2Z-UNC	-37.828 005 35	-37.775 321 18	0.052 684 170	11 562.839
	FCI	3Z	-37.848 854	crashed		
X2C,CN - NR,CN	CCSD	aCV4Z-UNC	-0.015 143 287	-0.015 154 977	-0.000 011 690	-2.57
	CCSD	aCV5Z-UNC	-0.015 159 821	-0.015 171 469	-0.000 011 648	-2.56
	CCSDT	aCV2Z-UNC	-0.015	-0.015	-0.000	-3.83
	CCSDT	aCV3Z-UNC	-0.015	-0.015	-0.000	-3.45
	CCSDT	aCV4Z-UNC	-0.015 141 997	-0.015 157 611	-0.000 015 614	-3.43
	CCSDT	aCV5Z-UNC	-0.015 158 538	-0.015 174 117	-0.000 015 579	-3.42
	CCSDTQ	aCV2Z-UNC				-3.13
	CCSDTQ	aCV3Z-UNC	-0.015 088 066	-0.015 100 612	-0.000 012 546	-2.75
	CCSDTQ	aCV3Z-UNC	-0.015 088 066	-0.015 100 612	-0.000 012 546	-2.75
	CCSDTQ	aCV4-UNC	-0.015 141 949	-0.015 154 419	-0.000 012 470	-2.74
	CCSDTQP	aCV2Z-UNC				-3.12
	FCI	aCV2Z-UNC				-3.11

Best theory

10 191.4(9)

10 192.654

Table II. At the 1 cm^{-1} digit, it does not make a difference which basis set or correlation level we use, so we can just add -3 cm^{-1} to the FCI/aug-cc-pCV7Z energy.

Correlation level	Basis set	$2^2P \leftarrow 2^1D$ energies for carbon			
		E_{NR} cm^{-1}	E_{X2C} cm^{-1}	$E_{\text{X2C-NR}}$ cm^{-1}	$E_{\text{X2C-NR}}$ rounded cm^{-1}
CCSD	aug-cc-pCV4Z-UNC	12 160.140	12 157.574	-2.57	-3
CCSD	aug-cc-pCV5Z-UNC	12 108.710	12 106.153	-2.56	-3
CCSDT	aug-cc-pCV2Z-UNC	12 398.642	12394.817	-3.83	-3
CCSDT	aug-cc-pCV3Z-UNC	11 348.625	11 345.170	-3.45	-3
CCSDT	aug-cc-pCV4Z-UNC	11 149.812	11 146.385	-3.43	-3
CCSDT	aug-cc-pCV5Z-UNC	11 080.842	11 077.422	-3.42	-3
CCSDTQ	aug-cc-pCV2Z-UNC	11 575.821	11 572.695	-3.13	-3
CCSDTQ	aug-cc-pCV3Z-UNC	10 522.186	10 519.433	-2.75	-3
CCSDTQ	aug-cc-pCV4Z-UNC	10 324.664	10 321.927	-2.75	-3
CCSDTQ	aug-cc-pCV5Z-UNC	10 256.915		-2.74	-3
CCSDTQP	aug-cc-pCV2Z-UNC	11 566.034	11 562.918	-3.12	-3
CCSDTQP	aug-cc-pCV5Z-UNC				
FCI	aug-cc-pCV2Z-UNC	11 565.947	11562.839	-3.11	-3
FCI	aug-cc-pCV3Z-UNC				