

	Total Energy	Energy above CCSDTQ
aug-cc-pCV2Z-NR		
Total CCSD energy [au]:	-14.933531 701417	
Total CCSD(T) energy [au]:	-14.933568 440497	
Total CCSDT energy [au]:	-14.933575 346708	458 nH
Total CCSDT(Q)/A energy [au]:	-14.933575 724924	
Total CCSDT(Q)/B energy [au]:	-14.933575 725169	94 nH
Total CCSDTQ energy [au]:	-14.933575 804573	0 uH
Total CCSDTQ(P)/A energy [au]:	-14.933575 804686	
Total CCSDTQ(P)/B energy [au]:	-14.933575 804687	
Total CCSDTQP energy [au]:	-14.933575 804716	
Total CCSDTQP(H)/A energy [au]:	-14.933575 804716	
Total CCSDTQP(H)/B energy [au]:	-14.933575 804716	
Total FCI energy [au]:	-14.933575 804743	
aug-cc-pCV3Z-NR		
Total CCSD energy [au]:	-14.949982 001939	
Total CCSD(T) energy [au]:	-14.950069 131674	
Total CCSDT energy [au]:	-14.950084 980481	781 nH
Total CCSDT(Q)/A energy [au]:	-14.950085 635194	
Total CCSDT(Q)/B energy [au]:	-14.950085 641049	120 nH
Total CCSDTQ energy [au]:	-14.950085 761173	000 nH
Total CCSDTQ(P)/A energy [au]:	-14.950085 761634	
Total CCSDTQ(P)/B energy [au]:	-14.950085 761637	
aug-cc-pCV4Z-NR		
Total CCSD energy [au]:	-14.954127 760323	
Total CCSD(T) energy [au]:	-14.954246 343848	
Total CCSDT energy [au]:	-14.954266 400787	893 nH
Total CCSDT(Q)/A energy [au]:	-14.954267 138736	
Total CCSDT(Q)/B energy [au]:	-14.954267 148074	146 nH
Total CCSDTQ energy [au]:	-14.954267 294251	000 nH
aug-cc-pCV5Z-NR		
Total CCSD energy [au]:	-14.956239 235626	
Total CCSD(T) energy [au]:	-14.956364 644050	
Total CCSDT energy [au]:	-14.956384 374501	875 nH
Total CCSDT(Q)/A energy [au]:	-14.956385 126463	
Total CCSDT(Q)/B energy [au]:	-14.956385 136054	114 nH
Total CCSDTQ energy [au]:	-14.956385 25	000 nH
aug-cc-pCV5Z-NR		
CCSD/CFOUR	-14.956239 082231	
CCSD(T)/CFOUR	-14.956364 490584	
CCSDT/CFOUR	-14.956384 221664	
CCSDT/CFOUR-MRCC	-14.956384 212115	(9 nH too high)
CCSDT(Q)/A/CFOUR-MRCC		
CCSDT(Q)/B/CFOUR-MRCC		
aug-cc-pCV6Z-NR		
CCSD/CFOUR	-14.956808 832727	
CCSD/CFOUR-MRCC	-14.956808 418226	
CCSD(T)/CFOUR	-14.956937 682317	
CCSD(T)/CFOUR-MRCC	-14.956937 267989	
CCSDT/CFOUR/est.	-14.956956 778477	850(60) nH [est. from -14.956956364477-4.14e-7]
CCSDT/CFOUR-MRCC	-14.956956 363028	
CCSDT(Q)/B/CFOUR/est.	-14.956957 553395	127(17) nH [est. from -14.956957139395-4.14e-7]
CCSDT(Q)/A/CFOUR-MRCC	-14.956957 129722	
CCSDT(Q)/B/CFOUR-MRCC	-14.956957 139395	
CCSDTQ/CFOUR-MRCC(est.)	-14.956957 628(060)	From -14.956956778477-850e-9
CCSDTQ/CFOUR-MRCC(est.)	-14.956957 680(017)	From -14.956957553395-127e-9
CCSDTQ/CFOUR-MRCC(est.)	-14.956957 680(060)	Conservative uncertainty estimate of 0.012 cm-1
aug-cc-pCV7Z-NR		
ROHF-CCSD/CFOUR		
ROHF-CCSD(T)/CFOUR		
CROHF-CCSDT/CFOUR	-14.957141 010744	
ROHF-CCSDTQ/CFOUR(est.)	-14.957141 860743	From 850(60)
UHF-CCSD/CFOUR		
UHF-CCSD(T)/CFOUR		
UHF-CCSDT/CFOUR	-14.957211 341106	
UHF-CCSDTQ/CFOUR(est.)	-14.957212 191106	From 850(60)
5Z: (-14.956385096+2*7.477431653828)*219474.6313705 = -333.9939358233644		
6Z: (-14.956957735+2*7.477718152465)*219474.6313705 = -333.9153037691335		
7Z: (-14.957211357355+2*7.477845563857)*219474.6313705 = -333.65184005712 (ROHF-based)		
7Z: (-14.957212191106+2*7.477845563857)*219474.6313705 = -333.8348272506497 (UHF-based)		
7Z: (-14.957212191106+2*7.477845563857)*219474.6313705 = -333.8348272506497 (UHF-based, with MRCC atomic)		