

Supporting information for: Accurate Calculation of the Dissociation Energy of the Highly Anharmonic System ClHCl^-

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Table 1: SCF, CCSD and (T) contributions to D_e (in cm^{-1}) as obtained by $\text{AV}n(+\text{d})\text{Z}/\text{V}n\text{Z}$ and $\text{AV}n(+\text{d})\text{Z}$ basis set combinations.

$\text{AV}n(+\text{d})\text{Z}/\text{V}n\text{Z}$						
	SCF		CCSD		(T)	
n	CP uncorr.	CP corr.	CP uncorr.	CP corr.	CP uncorr.	CP corr.
4	5009.6	5004.8	2456.2	2294.0	600.1	580.7
5	4997.0	4995.7	2505.1	2405.4	613.3	602.1
6	4989.3	4988.9	2516.0	2464.1	617.1	611.4
7	4987.9	4987.6	2525.7	2488.8	619.2	615.3
8	4987.5	4987.4	2531.9	2501.5	619.9	617.0

$\text{AV}n(+\text{d})\text{Z}$						
	SCF		CCSD		(T)	
n	CP uncorr.	CP corr.	CP uncorr.	CP corr.	CP uncorr.	CP corr.
4	5011.2	5006.7	2547.5	2313.7	613.1	586.1
5	4997.3	4995.5	2565.1	2415.3	620.9	604.7
6	4989.4	4989.0	2543.7	2470.3	620.5	612.7
7	4987.9	4987.7	2543.7	2491.1	621.0	615.8
8	4987.4	4987.4	2542.1	2501.3	620.8	617.2

Table 2: SCF, CCSD-F12b and (T) contributions to D_e (in cm^{-1}) as obtained by $\text{AV}n(+\text{d})\text{Z}/\text{V}n\text{Z}$ and $\text{AV}n(+\text{d})\text{Z}$ basis set combinations with corresponding OPTRI, JKFIT and MP2FIT auxiliary basis sets.

$\text{AV}n(+\text{d})\text{Z}/\text{V}n\text{Z}$						
	SCF		CCSD		(T)	
n	CP uncorr.	CP corr.	CP uncorr.	CP corr.	CP uncorr.	CP corr.
3	5048.5	5029.6	2478.3	2346.6	557.2	515.0
4	5009.6	5004.8	2532.3	2502.3	595.7	573.9
5	4997.0	4995.7	2536.5	2522.3	611.1	597.9

$\text{AV}n(+\text{d})\text{Z}$						
	SCF		CCSD		(T)	
n	CP uncorr.	CP corr.	CP uncorr.	CP corr.	CP uncorr.	CP corr.
3	5055.0	5032.7	2556.9	2371.7	581.4	526.5
4	5011.2	5006.7	2559.4	2510.4	609.6	579.2
5	4997.3	4995.5	2549.4	2524.4	619.8	600.4