

**Importance of electron correlation effects and basis set
superposition error in calculations of interaction energies and
interaction induced electric properties in hydrogen–bonded
complexes. A model study.**

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TABLE I: The counterpoise corrected finite field induced static electric dipole moment $\Delta\mu(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in au.

n	Method	LPol-ds	LPol-fs	LPol-dl	LPol-fl
2	HF SCF	0.305 (0.305)	0.306 (0.306)	0.306 (0.306)	0.306 (0.306)
	MP2	0.285 (0.285)	0.286 (0.286)	0.285 (0.285)	0.286 (0.286)
	CCSD	0.290 (0.290)	0.291 (0.291)	0.290 (0.290)	0.291 (0.292)
	CCSD(T)	0.292 (0.292)	0.293 (0.293)	0.292 (0.292)	0.293 (0.293)
3	HF SCF	0.713 (0.714)	0.715 (0.715)	0.715 (0.715)	0.716 (0.716)
	MP2	0.667 (0.667)	0.669 (0.668)	0.667 (0.667)	0.669 (0.669)
	CCSD	0.679 (0.679)	0.681 (0.682)	0.679 (0.680)	0.682 (0.682)
	CCSD(T)	0.683 (0.684)	0.686 (0.686)	0.684 (0.684)	0.686 (0.686)
4	HF SCF	1.165 (1.166)	1.169 (1.168)	1.168 (1.168)	1.170 (1.169)
	MP2	1.088 (1.088)	1.092 (1.091)	1.089 (1.089)	1.092 (1.091)
	CCSD	1.108 (1.109)	1.112 (1.113)	1.109 (1.110)	1.113 (1.113)
	CCSD(T)	1.116 (1.117)	1.120 (1.121)	1.117 (1.117)	1.121 (1.121)

TABLE II: The counterpoise corrected finite field induced static electric dipole polarizability $\Delta\alpha_{zz}(0)$ in the $(\text{HCN})_m$ ($m= 2 - 4$) complexes. The non-corrected values in parentheses. All results in au.

n	Method	LPol-ds		LPol-fs		LPol-dl		LPol-fl	
2	HF SCF	4.22	(4.21)	4.22	(4.24)	4.22	(4.23)	4.23	(4.23)
	MP2	4.28	(4.28)	4.31	(4.31)	4.29	(4.30)	4.31	(4.31)
	CCSD	4.35	(4.34)	4.37	(4.37)	4.35	(4.36)	4.37	(4.37)
	CCSD(T)	4.47	(4.46)	4.50	(4.49)	4.47	(4.48)	4.50	(4.49)
3	HF SCF	9.83	(9.83)	9.85	(9.87)	9.85	(9.87)	9.86	(9.87)
	MP2	10.00	(10.00)	10.06	(10.07)	10.02	(10.04)	10.08	(10.08)
	CCSD	10.16	(10.15)	10.21	(10.21)	10.18	(10.19)	10.22	(10.21)
	CCSD(T)	10.45	(10.44)	10.51	(10.51)	10.46	(10.47)	10.52	(10.51)
4	HF SCF	16.06	(16.05)	16.09	(16.12)	16.09	(16.13)	16.11	(16.13)
	MP2	16.36	(16.35)	16.45	(16.46)	16.39	(16.41)	16.48	(16.48)
	CCSD	16.62	(16.60)	16.70	(16.69)	16.64	(16.66)	16.71	(16.70)
	CCSD(T)	17.09	(17.07)	17.20	(17.18)	17.12	(17.13)	17.21	(17.20)

TABLE III: The counterpoise corrected finite field induced static electric dipole polarizability $\Delta\alpha_{xx}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in au.

n	Method	LPol-ds	LPol-fs	LPol-dl	LPol-fl
2	HF SCF	-0.94 (-0.94)	-0.94 (-0.94)	-0.94 (-0.95)	-0.94 (-0.94)
	MP2	-0.95 (-0.95)	-0.96 (-0.96)	-0.94 (-0.95)	-0.96 (-0.96)
	CCSD	-0.94 (-0.94)	-0.95 (-0.95)	-0.94 (-0.94)	-0.94 (-0.95)
	CCSD(T)	-0.96 (-0.96)	-0.96 (-0.97)	-0.95 (-0.96)	-0.96 (-0.97)
3	HF SCF	-2.08 (-2.07)	-2.07 (-2.07)	-2.08 (-2.09)	-2.07 (-2.07)
	MP2	-2.09 (-2.09)	-2.11 (-2.12)	-2.09 (-2.10)	-2.11 (-2.11)
	CCSD	-2.07 (-2.08)	-2.09 (-2.10)	-2.07 (-2.08)	-2.08 (-2.09)
	CCSD(T)	-2.11 (-2.12)	-2.13 (-2.14)	-2.10 (-2.12)	-2.12 (-2.13)
4	HF SCF	-3.27 (-3.26)	-3.26 (-3.26)	-3.27 (-3.29)	-3.26 (-3.26)
	MP2	-3.29 (-3.30)	-3.33 (-3.34)	-3.29 (-3.30)	-3.32 (-3.33)
	CCSD	-3.26 (-3.27)	-3.29 (-3.30)	-3.25 (-3.27)	— (—)
	CCSD(T)	-3.33 (-3.33)	-3.35 (-3.37)	-3.31 (-3.33)	— (—)

TABLE IV: The counterpoise corrected finite field induced static electric dipole first hyperpolarizability $\Delta\beta_{zzz}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in au.

n	Method	LPol-ds		LPol-fs		LPol-dl		LPol-fl	
2	HF SCF	22.8	(22.9)	22.7	(23.1)	22.7	(23.1)	22.8	(22.8)
	MP2	36.1	(36.4)	36.2	(36.5)	36.2	(36.5)	36.3	(36.2)
	CCSD	35.3	(35.6)	35.2	(35.4)	35.3	(35.6)	35.4	(35.2)
	CCSD(T)	37.3	(37.5)	37.2	(37.3)	37.3	(37.6)	37.3	(37.1)
3	HF SCF	57.7	(57.7)	57.5	(58.3)	57.5	(58.4)	57.7	(57.5)
	MP2	90.8	(91.4)	91.1	(91.6)	91.0	(91.8)	91.3	(91.0)
	CCSD	88.8	(89.2)	88.8	(89.1)	88.8	(89.4)	88.6	(88.2)
	CCSD(T)	94.1	(94.5)	94.0	(94.4)	94.1	(94.7)	93.9	(93.5)
4	HF SCF	98.6	(98.6)	98.4	(99.5)	98.4	(99.7)	98.6	(98.3)
	MP2	154.9	(155.6)	155.3	(156.1)	155.2	(156.3)	155.7	(155.2)
	CCSD	151.3	(151.9)	150.9	(151.4)	151.4	(152.3)	150.8	(150.2)
	CCSD(T)	160.5	(161.2)	160.2	(160.7)	160.7	(161.7)	160.2	(159.5)

TABLE V: The counterpoise corrected finite field induced static electric dipole first hyperpolarizability $\Delta\beta_{zxx}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in au.

n	Method	LPol-ds	LPol-fs	LPol-dl	LPol-fl
2	HF SCF	1.4 (1.5)	1.4 (1.1)	1.4 (1.5)	1.5 (1.5)
	MP2	1.0 (1.1)	1.2 (1.0)	1.1 (1.1)	1.2 (1.2)
	CCSD	0.9 (0.9)	1.1 (0.8)	1.0 (1.0)	1.1 (1.1)
	CCSD(T)	0.9 (1.0)	1.2 (0.8)	1.1 (1.1)	1.2 (1.2)
3	HF SCF	3.0 (3.1)	3.0 (2.4)	3.0 (3.2)	3.1 (3.1)
	MP2	2.0 (2.1)	2.4 (1.9)	2.2 (2.2)	2.4 (2.4)
	CCSD	1.7 (1.7)	1.9 (1.4)	1.9 (2.0)	2.0 (2.0)
	CCSD(T)	1.9 (1.9)	2.1 (1.6)	2.0 (2.1)	2.2 (2.2)
4	HF SCF	4.5 (4.8)	4.7 (3.8)	4.7 (5.0)	4.8 (4.7)
	MP2	3.0 (3.1)	3.6 (2.9)	3.2 (3.4)	3.6 (3.6)
	CCSD	2.4 (2.4)	2.8 (2.1)	2.7 (2.9)	— (—)
	CCSD(T)	2.5 (2.6)	3.1 (2.4)	3.0 (3.1)	— (—)

TABLE VI: The counterpoise corrected finite field induced static electric dipole second hyperpolarizability $\Delta\gamma_{zzzz}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in 10^3 au.

n	Method	LPol-ds	LPol-fs	LPol-dl	LPol-fl
2	HF SCF	1.00 (1.05)	0.99 (1.01)	1.00 (1.04)	1.01 (1.00)
	MP2	1.42 (1.47)	1.43 (1.44)	1.42 (1.47)	1.45 (1.44)
	CCSD	1.36 (1.40)	1.51 (1.51)	1.36 (1.40)	1.36 (1.35)
	CCSD(T)	1.54 (1.58)	1.70 (1.70)	1.54 (1.58)	1.55 (1.53)
3	HF SCF	2.51 (2.59)	2.50 (2.53)	2.51 (2.58)	2.53 (2.51)
	MP2	3.61 (3.71)	3.62 (3.65)	3.58 (3.66)	3.65 (3.63)
	CCSD	3.45 (3.52)	3.41 (3.42)	3.45 (3.51)	3.43 (3.41)
	CCSD(T)	3.90 (3.98)	3.87 (3.89)	3.90 (3.97)	3.90 (3.88)
4	HF SCF	4.29 (4.40)	4.28 (4.33)	4.29 (4.40)	4.31 (4.29)
	MP2	6.16 (6.29)	6.22 (6.27)	6.18 (6.29)	6.26 (6.23)
	CCSD	5.89 (5.99)	6.15 (6.17)	5.83 (5.93)	6.10 (6.09)
	CCSD(T)	6.68 (6.79)	6.98 (7.00)	6.62 (6.73)	6.91 (6.91)

TABLE VII: The counterpoise corrected finite field induced static electric dipole second hyperpolarizability $\Delta\gamma_{xxxx}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in 10^3 au.

n	Method	LPol-ds	LPol-fs	LPol-dl	LPol-fl
2	HF SCF	-0.32 (-0.30)	-0.37 (-0.39)	-0.31 (-0.30)	-0.36 (-0.37)
	MP2	-0.32 (-0.29)	-0.36 (-0.38)	-0.31 (-0.29)	-0.36 (-0.36)
	CCSD	-0.31 (-0.29)	-0.40 (-0.38)	-0.30 (-0.29)	-0.32 (-0.33)
	CCSD(T)	-0.33 (-0.30)	-0.43 (-0.40)	-0.32 (-0.31)	-0.33 (-0.35)
3	HF SCF	-0.71 (-0.66)	-0.81 (-0.85)	-0.70 (-0.66)	-0.80 (-0.82)
	MP2	-0.70 (-0.65)	-0.80 (-0.84)	-0.70 (-0.66)	-0.79 (-0.81)
	CCSD	-0.69 (-0.64)	-0.56 (-0.59)	-0.67 (-0.64)	-0.87 (-0.88)
	CCSD(T)	-0.73 (-0.68)	-0.60 (-0.63)	-0.72 (-0.68)	-0.93 (-0.93)
4	HF SCF	-1.12 (-1.05)	-1.27 (-1.33)	-1.09 (-1.04)	-1.26 (-1.29)
	MP2	-1.11 (-1.03)	-1.26 (-1.31)	-1.08 (-1.02)	-1.25 (-1.27)
	CCSD	-1.04 (-0.96)	-1.19 (-1.23)	-1.08 (-1.02)	— (—)
	CCSD(T)	-1.11 (-1.03)	-1.26 (-1.32)	-1.15 (-1.08)	— (—)

TABLE VIII: The counterpoise corrected finite field induced static electric dipole second hyperpolarizability $\Delta\gamma_{xxzz}(0)$ in the $(\text{HCN})_m$ ($m=2-4$) complexes. The non-corrected values in parentheses. All results in 10^3 au.

n	Method	LPol-ds		LPol-fs		LPol-dl		LPol-fl	
2	HF SCF	0.00	(0.00)	0.00	(0.00)	0.00	(0.01)	0.00	(0.00)
	MP2	-0.01	(-0.01)	-0.01	(-0.01)	-0.01	(0.00)	-0.01	(-0.02)
	CCSD	0.01	(0.02)	0.10	(0.14)	-0.01	(-0.01)	0.03	(0.03)
	CCSD(T)	0.01	(0.02)	0.10	(0.15)	-0.01	(0.00)	0.04	(0.04)
3	HF SCF	0.00	(0.02)	-0.01	(0.00)	-0.01	(0.01)	-0.01	(-0.01)
	MP2	0.00	(0.02)	-0.04	(-0.03)	-0.05	(-0.03)	-0.04	(-0.04)
	CCSD	-0.03	(-0.02)	0.07	(0.07)	-0.04	(-0.02)	-0.11	(-0.12)
	CCSD(T)	-0.03	(-0.01)	0.08	(0.09)	-0.03	(-0.01)	-0.11	(-0.11)
4	HF SCF	-0.01	(0.01)	-0.01	(0.01)	0.00	(0.03)	-0.01	(-0.02)
	MP2	-0.06	(-0.03)	-0.06	(-0.05)	-0.05	(-0.02)	-0.05	(-0.07)
	CCSD	-0.04	(-0.01)	-0.04	(-0.03)	-0.09	(-0.06)	—	(—)
	CCSD(T)	-0.03	(-0.01)	-0.03	(-0.02)	-0.09	(-0.05)	—	(—)

TABLE IX: The counterpoise corrected interaction energy $\Delta E(0)$ in the $(\text{HCN})_m$ ($m= 2 - 4$) complexes. The non-corrected values in parentheses. All results in kcal mol⁻¹.

n	Method	LPol-ds		LPol-fs		LPol-dl		LPol-fl	
2	HF SCF	-4.07	(-4.15)	-4.10	(-4.34)	-4.09	(-4.11)	-4.11	(-4.24)
	MP2	-4.59	(-5.56)	-4.67	(-6.62)	-4.61	(-5.22)	-4.69	(-5.82)
	CCSD	-4.29	(-5.16)	-4.38	(-6.14)	-4.31	(-4.82)	-4.40	(-5.45)
	CCSD(T)	-4.39	(-5.32)	-4.49	(-6.36)	-4.41	(-4.96)	-4.51	(-5.62)
3	HF SCF	-9.13	(-9.29)	-9.20	(-9.71)	-9.17	(-9.21)	-9.21	(-9.50)
	MP2	-10.21	(-12.22)	-10.40	(-14.50)	-10.26	(-11.48)	-10.44	(-12.91)
	CCSD	-9.55	(-11.36)	-9.76	(-13.46)	-9.61	(-10.61)	-9.81	(-12.11)
	CCSD(T)	-9.77	(-11.70)	-10.02	(-13.96)	-9.83	(-10.92)	-10.07	(-12.50)
4	HF SCF	-14.41	(-14.66)	-14.53	(-15.32)	-14.48	(-14.55)	-14.54	(-14.99)
	MP2	-16.20	(-19.30)	-16.51	(-22.79)	-16.28	(-18.16)	-16.57	(-20.41)
	CCSD	-15.11	(-17.90)	-15.47	(-21.13)	-15.20	(-16.76)	-15.54	(-19.13)
	CCSD(T)	-15.49	(-18.47)	-15.90	(-21.94)	-15.59	(-17.26)	-15.98	(-19.76)