

TABLES

TABLE I. Cholesky decompositions with threshold 10^{-8} . Actual number of shell distributions is the *unique* number of distributions calculated.

Molecule	Group	Basis Set	N	Cholesky Vectors		Shell Distributions	
				Max.	Actual	Max.	Actual
Benzene	D_{2h}	6-31G	66	2211	927	21	20
		6-31++G	96	4656	1240	21	20
		aug-cc-pVDZ	192	18528	2632	55	45
		aug-cc-pVTZ	414	85905	5869	105	74
		aug-cc-pVQZ	756	286146	11121	171	114
		aug-cc-pCVDZ	216	23436	2873	55	42
		aug-cc-pCVTZ	492	121278	6937	105	75
TCO (C_8H_{14})	C_2	6-31G	100	5050	1486	120	78
		6-31++G	146	10731	1880	120	74
		aug-cc-pVDZ	310	48205	3989	351	162
		aug-cc-pVTZ	690	238395	9227	703	246
		aug-cc-pCVDZ	342	58653	4310	351	157
		aug-cc-pCVTZ	794	315615	10371	703	226
Stilbene I ($C_{14}N_2H_{14}$)	C_1	6-31G	172	14878	2131	1081	224
		6-31++G	250	31375	2722	1081	233
		aug-cc-pVDZ	494	122265	5864	2926	505
Stilbene II ($C_{46}N_2H_{36}$)	C_1	6-31G [seg.]	504	127260	6301	48828	2159
		6-31++G [seg.]	732	268278	7574	98790	2640
		aug-cc-pVDZ [seg.]	1428	1020306	16726	187578	2554
C_{60}	D_{2h}	6-31G	540	146070	9226	171	76
		6-31++G	780	304590	10532	171	73
		aug-cc-pVDZ [seg.]	1380	952890	19714	3321	302

TABLE II. CO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF convergence was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
aug-cc-pV5Z (254)	10^{-3}	7.3	16.1	-0.5×10^{-3}
	10^{-4}	8.6	15.2	-0.3×10^{-4}
	10^{-5}	9.8	12.8	-0.6×10^{-5}
	10^{-6}	11.0	11.1	-1.6×10^{-6}
	10^{-7}	12.2	10.4	-0.8×10^{-7}
	10^{-8}	13.4	9.2	-0.3×10^{-8}
aug-cc-pCV5Z (342)	10^{-3}	7.7	37.0	4.7×10^{-6}
	10^{-4}	9.0	29.4	2.3×10^{-6}
	10^{-5}	10.3	26.8	1.8×10^{-6}
	10^{-6}	11.5	24.7	3.9×10^{-9}
	10^{-7}	12.7	22.6	1.2×10^{-9}
	10^{-8}	13.9	17.8	0.9×10^{-9}

TABLE III. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
aug-cc-pVDZ (192)	10^{-3}	4.2	15.0	-0.9×10^{-3}
	10^{-4}	5.6	12.8	-0.8×10^{-4}
	10^{-5}	7.2	9.1	-1.5×10^{-5}
	10^{-6}	9.3	7.1	-0.1×10^{-6}
	10^{-7}	11.6	5.3	-0.1×10^{-7}
	10^{-8}	13.7	4.9	-0.2×10^{-8}
aug-cc-pCVDZ (216)	10^{-3}	4.2	16.3	-0.4×10^{-3}
	10^{-4}	5.7	12.3	0.4×10^{-5}
	10^{-5}	7.1	10.9	-0.3×10^{-7}
	10^{-6}	9.0	7.5	-0.4×10^{-6}
	10^{-7}	11.2	6.1	-0.8×10^{-7}
	10^{-8}	13.3	6.1	-2.6×10^{-8}

TABLE IV. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	pJ	τ	ΔE
aug-cc-pVTZ (414)	10^{-3}	5.3	51.5	-0.7×10^{-3}
	10^{-4}	6.7	40.7	-1.3×10^{-4}
	10^{-5}	8.3	33.4	-0.5×10^{-5}
	10^{-6}	10.1	25.1	-0.6×10^{-6}
	10^{-7}	11.9	19.4	-0.5×10^{-7}
	10^{-8}	14.2	16.4	-1.4×10^{-8}
aug-cc-pCVTZ (492)	10^{-3}	5.4	64.9	-0.1×10^{-3}
	10^{-4}	6.8	50.7	0.1×10^{-4}
	10^{-5}	8.1	40.5	-0.1×10^{-5}
	10^{-6}	9.9	30.7	-0.1×10^{-6}
	10^{-7}	11.9	24.8	-0.1×10^{-7}
	10^{-8}	14.1	19.9	-0.1×10^{-8}

TABLE V. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build); the Cholesky and integral–direct calculations were run on different machines, thus τ is not really well–defined (although the time of the integral–direct calculation has been corrected). Moreover, the integral–direct calculation was not allowed to use screening. In all calculations the threshold for SCF was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
aug-cc-pVQZ	10^{-4}	7.8	(1002)	-1.3×10^{-4}
(756, dir.)	10^{-5}	9.2	(899)	-2.6×10^{-5}
	10^{-6}	10.8	(750)	-0.8×10^{-6}
	10^{-7}	12.7	(651)	-1.5×10^{-7}
	10^{-8}	14.7	(545)	-1.0×10^{-8}

TABLE VI. N₂—Benzene van der Waals complex. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree, except interaction energy which is in cm⁻¹. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF convergence was 10⁻⁸.

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
Complex:				
aug-cc-pVDZ-33211 (276)	10 ⁻⁸	12.6	3.2	-0.8 × 10 ⁻⁸
Benzene CP:				
aug-cc-pVDZ-33211 (276)			3.4	-0.6 × 10 ⁻⁸
N ₂ CP:				
aug-cc-pVDZ-33211 (276)			5.7	-0.3 × 10 ⁻⁸
Int. Energy:				
aug-cc-pVDZ-33211 (276)				-4.4 × 10 ⁻⁴

TABLE VII. TCO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF convergence was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
aug-cc-pVDZ	10^{-3}	3.5	29.3	1.1×10^{-3}
(310)	10^{-4}	4.9	19.6	1.0×10^{-4}
	10^{-5}	6.2	15.4	2.9×10^{-5}
	10^{-6}	8.1	12.1	0.5×10^{-6}
	10^{-7}	10.4	8.9	0.2×10^{-7}
	10^{-8}	12.9	7.7	1.1×10^{-8}
aug-cc-pCVDZ	10^{-3}	3.5	29.3	-0.6×10^{-4}
(342)	10^{-4}	4.9	19.5	0.7×10^{-5}
	10^{-5}	6.2	12.2	0.4×10^{-6}
	10^{-6}	8.0	12.6	-0.6×10^{-6}
	10^{-7}	10.3	7.6	-2.2×10^{-7}
	10^{-8}	12.6	6.9	-4.3×10^{-8}

TABLE VIII. TCO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF convergence was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
aug-cc-pVTZ	10^{-6}	9.2	42.9	-2.6×10^{-6}
(690, dir.)	10^{-7}	11.1	37.9	-0.4×10^{-7}
	10^{-8}	13.4	27.1	-1.7×10^{-8}

TABLE IX. Stilbene I. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., Fock build). In all calculations the threshold for SCF convergence was 10^{-8} .

Basis Set	Cholesky		SCF	
	Threshold	p_J	τ	ΔE
6-31G (172)	10^{-8}	12.4	0.6	-2.2×10^{-7}
6-31++G (250)	10^{-8}	10.9	1.7	-2.1×10^{-7}
aug-cc-pVDZ (494, dir.)	10^{-8}	11.9	23.8	-1.6×10^{-8}

TABLE X. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$, where the conventional time is for calculating the $(ia|jb)$ integrals and the Cholesky time is for a full MP2 calculation. In all calculations the threshold for SCF convergence was 10^{-8} . All electrons correlated. “single dec.” means that only the original AO Cholesky vectors were used, whereas “double dec.” signifies that a separate $(ia|jb)$ decomposition was employed.

Basis Set	Cholesky Threshold	MP2 single dec.			MP2 double dec.		
		p_J	τ	ΔE	p_K	τ	ΔE
aug-cc-pVDZ (192)	10^{-3}	4.2	10.3	-1.3×10^{-3}	1.3	10.2	-6.8×10^{-3}
	10^{-4}	5.6	8.1	-1.3×10^{-4}	2.2	7.0	-4.1×10^{-4}
	10^{-5}	7.2	6.8	-2.1×10^{-5}	3.1	5.8	-4.5×10^{-5}
	10^{-6}	9.3	4.9	-0.6×10^{-6}	4.3	3.8	-2.2×10^{-6}
	10^{-7}	11.6	4.0	-0.4×10^{-7}	5.8	2.9	-1.9×10^{-7}
	10^{-8}	13.7	3.8	-0.7×10^{-8}	7.4	2.5	-2.7×10^{-8}
aug-cc-pCVDZ (216)	10^{-3}	4.2	12.6	-0.9×10^{-3}	1.3	12.7	-5.6×10^{-3}
	10^{-4}	5.7	10.5	-0.3×10^{-4}	2.2	9.6	-3.1×10^{-4}
	10^{-5}	7.1	8.0	-0.3×10^{-5}	3.0	7.2	-2.9×10^{-5}
	10^{-6}	9.0	5.9	-0.9×10^{-6}	4.1	5.8	-3.3×10^{-6}
	10^{-7}	11.2	5.0	-1.2×10^{-7}	5.4	3.6	-3.3×10^{-7}
	10^{-8}	13.3	4.6	-3.5×10^{-8}	7.1	3.4	-5.8×10^{-8}

TABLE XI. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$, where the conventional time is for calculating the $(ia|jb)$ integrals and the Cholesky time is for a full MP2 calculation. In all calculations the threshold for SCF convergence was 10^{-8} . All electrons correlated. “single dec.” means that only the original AO Cholesky vectors were used, whereas “double dec.” signifies that a separate $(ia|jb)$ decomposition was employed.

Basis Set	Cholesky Threshold	MP2 single dec.			MP2 double dec.		
		p_J	τ	ΔE	p_K	τ	ΔE
aug-cc-pVTZ (414)	10^{-3}	5.3	29.8	-1.2×10^{-3}	1.0	39.7	-1.5×10^{-2}
	10^{-4}	6.7	25.0	-3.6×10^{-4}	1.7	27.8	-1.2×10^{-3}
	10^{-5}	8.3	20.0	-5.7×10^{-5}	2.1	20.8	-1.1×10^{-4}
	10^{-6}	10.1	15.2	-7.0×10^{-6}	3.2	13.9	-1.2×10^{-5}
	10^{-7}	11.9	13.2	-5.8×10^{-7}	4.1	10.4	-9.7×10^{-7}
	10^{-8}	14.2	10.9	-7.1×10^{-8}	5.3	9.3	-1.2×10^{-7}
aug-cc-pCVTZ (492)	10^{-3}	5.4	30.3	-0.2×10^{-3}	0.9	43.0	-1.5×10^{-2}
	10^{-4}	6.8	23.4	-0.2×10^{-4}	1.7	30.4	-0.8×10^{-3}
	10^{-5}	8.1	19.7	-0.2×10^{-5}	2.3	20.6	-0.5×10^{-4}
	10^{-6}	9.9	15.8	-0.1×10^{-6}	3.1	16.1	-0.6×10^{-5}
	10^{-7}	11.9	14.1	-0.3×10^{-7}	4.0	13.4	-0.5×10^{-6}
	10^{-8}	14.1	10.9	-0.4×10^{-8}	5.1	10.6	-0.6×10^{-7}

TABLE XII. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$, where the conventional time is for calculating the $(ia|jb)$ integrals and the Cholesky time is for a full MP2 calculation; calculations performed on different machines, thus τ is merely an estimate. In all calculations the threshold for SCF convergence was 10^{-8} . All electrons correlated. “single dec.” means that only the original AO Cholesky vectors were used, whereas “double dec.” signifies that a separate $(ia|jb)$ decomposition was employed.

Basis Set	Cholesky Threshold	MP2 single dec.			MP2 double dec.		
		p_J	τ	ΔE	p_K	τ	ΔE
aug-cc-pVQZ (756, dir.)	10^{-4}	7.8	(1930)	-4.3×10^{-4}	1.4	(2704)	-1.6×10^{-3}
	10^{-5}	9.2	(1726)	-1.0×10^{-4}	2.0	(2228)	-2.0×10^{-4}
	10^{-6}	10.8	(1708)	-0.8×10^{-5}	2.7	(1994)	-1.6×10^{-5}
	10^{-7}	12.7	(1327)	-2.2×10^{-6}	3.3	(1383)	-2.8×10^{-6}
	10^{-8}	14.7	(1155)	-2.1×10^{-7}	4.0	(1163)	-2.7×10^{-7}

TABLE XIII. TCO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$, where the conventional time is for calculating the $(ia|jb)$ integrals and the Cholesky time is for a full MP2 calculation; calculations performed on different machines, thus τ is merely an estimate. In all calculations the threshold for SCF convergence was 10^{-8} . Frozen core calculation. “single dec.” means that only the original AO Cholesky vectors were used, whereas “double dec.” signifies that a separate $(ia|jb)$ decomposition was employed.

Basis Set	Cholesky Threshold	MP2 single dec.			MP2 double dec.		
		p_J	τ	ΔE	p_K	τ	ΔE
aug-cc-pVTZ	10^{-6}	9.2	87.8	-4.0×10^{-6}	2.7	131.7	-6.0×10^{-5}
(690, dir.)	10^{-7}	11.1	74.8	-0.9×10^{-7}	3.5	97.4	-4.9×10^{-6}
	10^{-8}	13.4	63.4	-2.5×10^{-8}	4.5	73.3	-4.7×10^{-7}

TABLE XIV. C_{60} . All electrons correlated. Energies in hartree, timings in hours.

Hardware: IBM p690 "Regatta", Power4, 5.2 Gflops (aug-cc-pVDZ calc.),

IBM RS/6000, Power3, 1.6 Gflops (6-31G and 6-31++G).

SCF convergence (gradient): 5.0×10^{-7} .

Basis	Cholesky		MP2 single dec.			MP2 double dec.			
	Set	N	Threshold	p_J	Time	E_{MP2}	p_K	Time	E_{MP2}
6-31G		540	10^{-8}	17.1	0.3	-2276.4414626697	10.6	0.3	-2276.4414616356
6-31++G		780	10^{-8}	13.5	0.9	-2276.6025044092	8.5	0.7	-2276.6025030641
aug-cc-pVDZ [seg.]		1380	10^{-8}	14.3	2.9	-2280.2239066115	7.0	1.8	-2280.2239016896

TABLE XV. CO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10^{-8} .

Basis Set	Cholesky		CC2	
	Threshold	pJ	τ	ΔE
aug-cc-pV5Z (254)	10^{-3}	7.3	26.6	-1.2×10^{-3}
	10^{-4}	8.6	21.9	-0.9×10^{-4}
	10^{-5}	9.8	20.0	-2.6×10^{-5}
	10^{-6}	11.0	17.5	-5.1×10^{-6}
	10^{-7}	12.2	16.2	-6.2×10^{-7}
	10^{-8}	13.4	13.8	-4.5×10^{-8}
aug-cc-pCV5Z (342)	10^{-3}	7.7	40.7	3.0×10^{-6}
	10^{-4}	9.0	30.5	1.3×10^{-6}
	10^{-5}	10.3	27.1	0.9×10^{-6}
	10^{-6}	11.5	26.6	1.8×10^{-8}
	10^{-7}	12.7	24.4	1.0×10^{-8}
	10^{-8}	13.9	19.5	1.0×10^{-8}

TABLE XVI. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10^{-8} .

Basis Set	Cholesky		CC2	
	Threshold	p_J	τ	ΔE
aug-cc-pVDZ (192)	10^{-3}	4.2	29.5	-1.3×10^{-3}
	10^{-4}	5.6	23.6	-1.3×10^{-4}
	10^{-5}	7.2	18.8	-2.0×10^{-5}
	10^{-6}	9.3	12.8	-0.6×10^{-6}
	10^{-7}	11.6	10.3	-0.4×10^{-7}
	10^{-8}	13.7	10.5	-0.7×10^{-8}
aug-cc-pCVDZ (216)	10^{-3}	4.2	37.5	-0.9×10^{-3}
	10^{-4}	5.7	28.6	-0.3×10^{-4}
	10^{-5}	7.1	21.6	-0.3×10^{-5}
	10^{-6}	9.0	16.7	-0.9×10^{-6}
	10^{-7}	11.2	13.3	-1.4×10^{-7}
	10^{-8}	13.3	13.3	-8.7×10^{-8}

TABLE XVII. Benzene. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10^{-8} .

Basis Set	Cholesky		CC2	
	Threshold	p_J	τ	ΔE
aug-cc-pVTZ (414)	10^{-3}	5.3	51.5	-1.2×10^{-3}
	10^{-4}	6.7	39.2	-3.6×10^{-4}
	10^{-5}	8.3	31.3	-5.7×10^{-5}
	10^{-6}	10.1	25.2	-7.0×10^{-6}
	10^{-7}	11.9	19.6	-5.8×10^{-7}
	10^{-8}	14.2	16.9	-6.8×10^{-8}
aug-cc-pCVTZ (492)	10^{-3}	5.4	55.4	-0.2×10^{-3}
	10^{-4}	6.8	43.3	-0.2×10^{-4}
	10^{-5}	8.1	31.6	-0.2×10^{-5}
	10^{-6}	9.9	29.1	-0.1×10^{-6}
	10^{-7}	11.9	23.0	-0.3×10^{-7}
	10^{-8}	14.1	19.1	-0.1×10^{-10}

TABLE XVIII. N₂—Benzene van der Waals complex. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree, except interaction energy which is in cm⁻¹. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10⁻⁸.

Basis Set	Cholesky		CC2	
	Threshold	p_J	τ	ΔE
Complex:				
aug-cc-pVDZ-33211 (276)	10 ⁻⁸	12.6	6.9	-3.4 × 10 ⁻⁸
Benzene CP:				
aug-cc-pVDZ-33211 (276)			7.7	-2.8 × 10 ⁻⁸
N ₂ CP:				
aug-cc-pVDZ-33211 (276)			18.9	0.7 × 10 ⁻⁸
Int. Energy:				
aug-cc-pVDZ-33211 (276)				2.9 × 10 ⁻³

TABLE XIX. TCO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10^{-8} . Frozen core approximation.

Basis Set	Cholesky		CC2	
	Threshold	p_J	τ	ΔE
aug-cc-pVDZ	10^{-3}	3.5	28.7	2.2×10^{-3}
(310)	10^{-4}	4.9	19.7	1.7×10^{-4}
	10^{-5}	6.2	15.1	3.9×10^{-5}
	10^{-6}	8.1	11.7	-2.3×10^{-6}
	10^{-7}	10.4	9.4	-1.0×10^{-7}
	10^{-8}	12.9	7.6	1.2×10^{-8}
aug-cc-pCVDZ	10^{-3}	3.5	28.9	-1.1×10^{-3}
(342)	10^{-4}	4.9	19.3	-0.6×10^{-4}
	10^{-5}	6.2	15.5	-1.0×10^{-5}
	10^{-6}	8.0	13.2	-1.7×10^{-6}
	10^{-7}	10.3	9.6	-3.2×10^{-7}
	10^{-8}	12.6	8.1	-6.8×10^{-8}

TABLE XX. TCO. $\Delta E = E_{\text{conventional}} - E_{\text{Cholesky}}$ in Hartree. $\tau = T_{\text{conventional}}/T_{\text{Cholesky}}$ for average iteration times (i.e., CC2 vector function). In all calculations the threshold for SCF and CC2 convergence was 10^{-8} . Frozen core approximation.

Basis Set	Cholesky		CC2	
	Threshold	p_J	τ	ΔE
aug-cc-pVTZ	10^{-6}	9.2	58.0	-3.3×10^{-6}
(690, dir.)	10^{-7}	11.1	48.2	-0.4×10^{-7}
	10^{-8}	13.4	40.8	-3.7×10^{-8}

TABLE XXI. C_{60} . All electrons correlated. Energies in hartree, average iteration times in hours.

Hardware: IBM RS/6000, Power3, 0.8 Gflops (aug-cc-pVDZ calc.),

IBM RS/6000, Power3, 1.6 Gflops (6-31G and 6-31++G).

SCF convergence (gradient): 5.0×10^{-7} , CC2 convergence (energy, gradient): 10^{-8} , 10^{-6} .

Basis	Cholesky		CC2 single dec.			CC2 double dec. (T_2)		
	Set	N	Threshold	p_J	Time	E_{CC2}	p_K	Time
6-31G	540	10^{-8}	17.1	0.7	-2276.5234782738	18.9	0.8	-2276.5234761610
6-31++G	780	10^{-8}	13.5	1.8	-2276.6874585388			
aug-cc-pVDZ	1380	10^{-8}	14.3	23.9	-2280.3533813134			