

Supporting Information

Big Data analysis of *ab initio* molecular integrals in the neglect of diatomic differential overlap approximation

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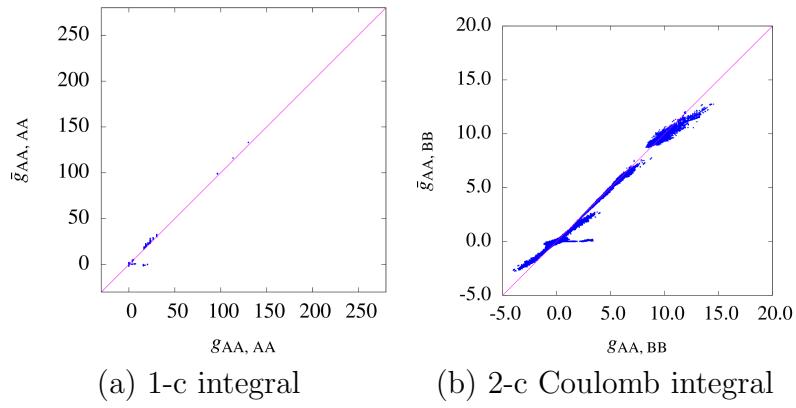


Figure S1: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron single- ζ STO-3G basis function is employed for integral evaluation.

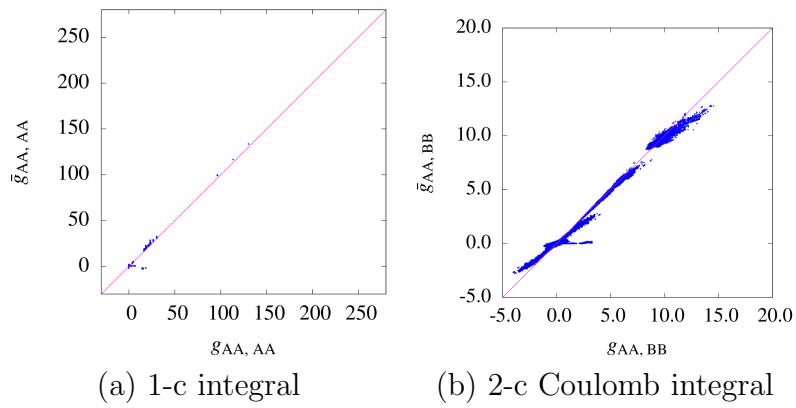


Figure S2: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron single- ζ STO-6G basis function is employed for integral evaluation.

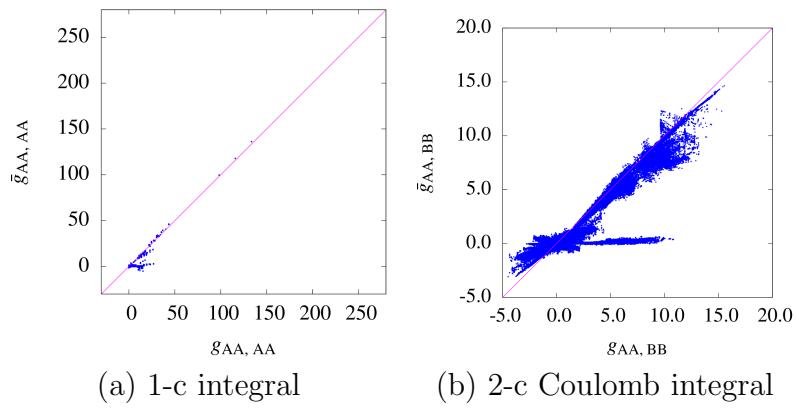


Figure S3: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron double- ζ 3-21G basis function is employed for integral evaluation.

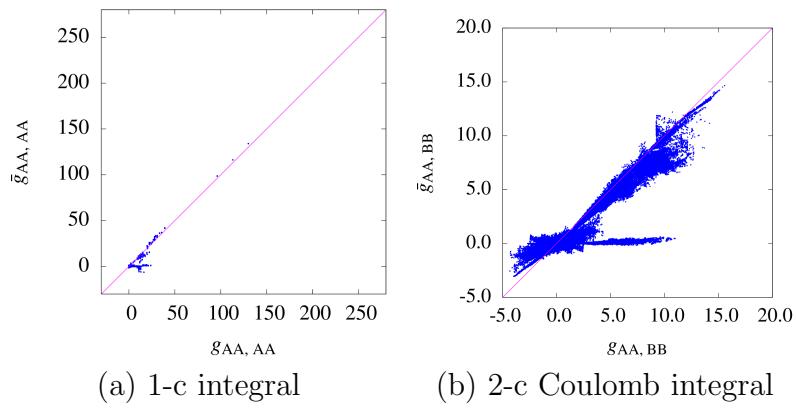


Figure S4: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron double- ζ 6-31G basis function is employed for integral evaluation.

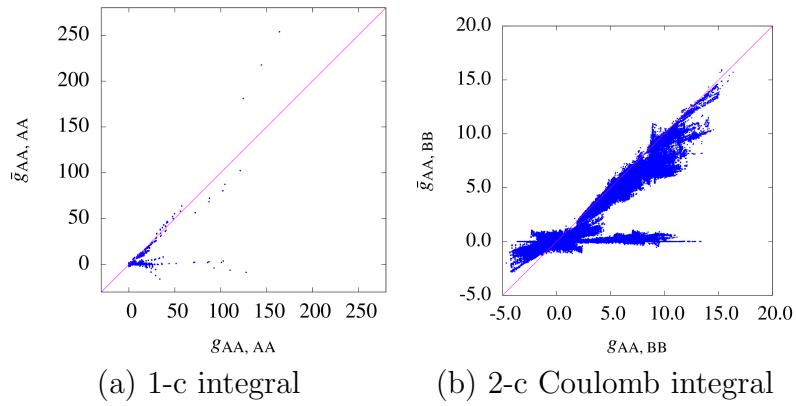


Figure S5: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation.

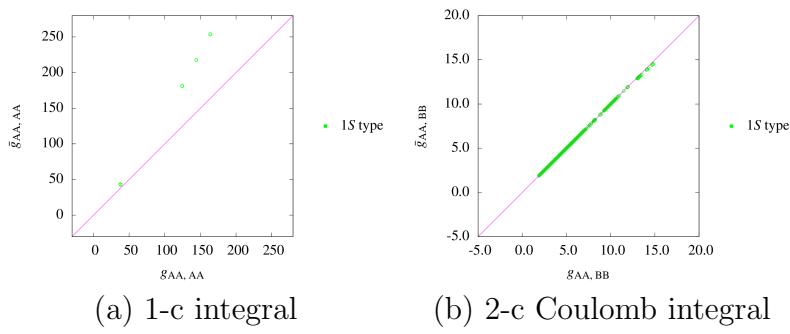


Figure S6: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. 1S type refer to the integrals involving purely the 1S shell, respectively.

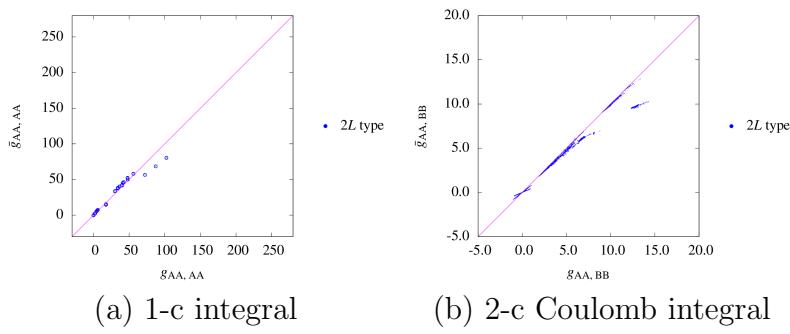


Figure S7: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. 2L type refer to the integrals involving purely the 2SP shell, respectively.

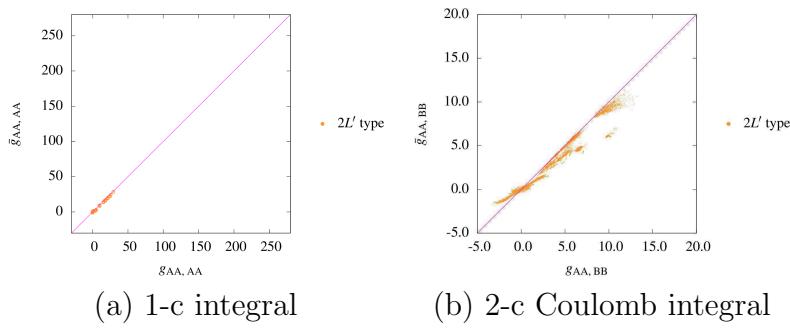


Figure S8: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. 2L' type refer to the integrals involving purely the 2S'P' shell, respectively.

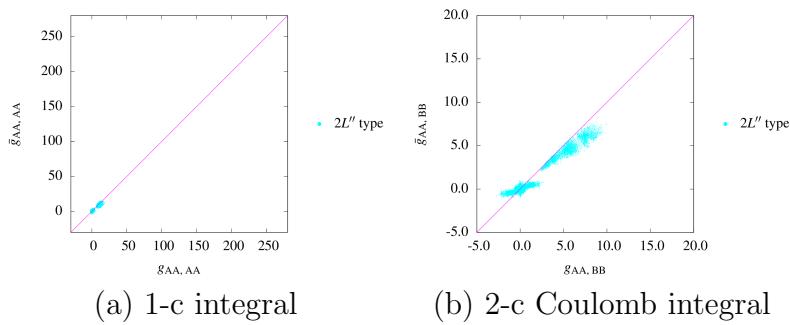


Figure S9: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. 2L'' type refer to the integrals involving purely the 2S''P'' shell, respectively.

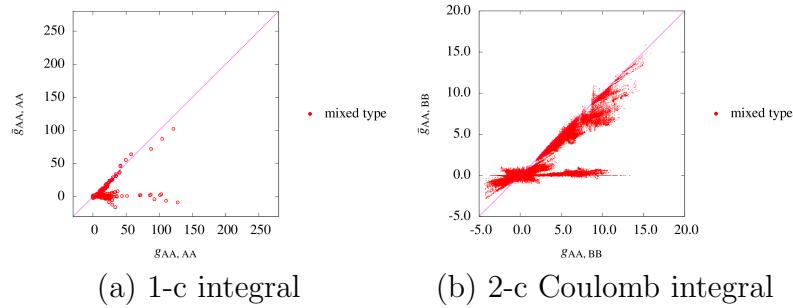


Figure S10: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. The mixed type of Coulomb integrals involves basis functions in different shells.

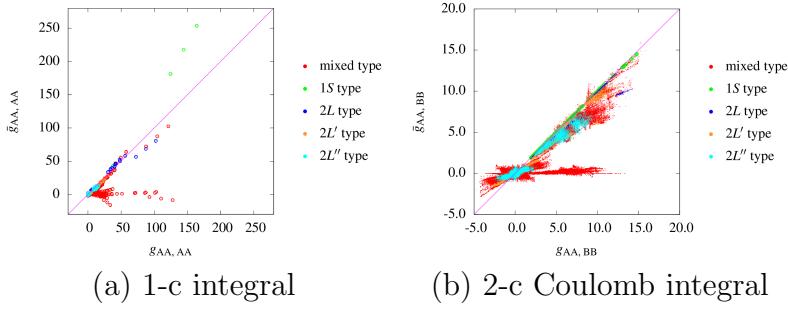


Figure S11: Correlation diagrams of the NDDO-retained *ab initio* 2-e Coulomb type integrals (all in eV) in the atomic basis (abscissa) and the Löwdin basis (ordinate). The all-electron triple- ζ 6-311G basis function is employed for integral evaluation. 1S, 2L, 2L', and 2L'' types refer to the integrals involving purely the 1S, 2SP, 2S'P', and 2S''P'' shells, respectively. The mixed type of Coulomb integrals involves basis functions in different shells.

GTO	NDDO-retained		NDDO-neglected				
	Coulomb integral		exchange integral			hybrid integral	
	g_{1cc}	g_{2cc}	g_{2cx}	g_{3cx}	g_{4cx}	g_{2ch}	g_{3ch}
CEP-4G	52228	399096	798192	18165696	54030408	1861488	9082848
STO-3G	127135	919314	1838628	38685112	106781232	4266376	19342556
STO-6G	127135	919314	1838628	38685112	106781232	4266376	19342556
3-21G	1336043	9889712	19779424	431576040	1233229392	46053896	215788020
6-31G	1336043	9889712	19779424	431576040	1233229392	46053896	215788020
6-311G	5389556	36928164	73856328	1444980096	3484427568	173624256	722490048
sum	8368140	58945312	117890624	2403668096	6218479224	276126288	1201834048

Table S1: The number of every type of *ab initio* 2-e integrals in different GTO basis sets for the Big Data analysis. The total number of 2-e integrals is approximately 10.3 billion.

GTO	NDDO-retained			NDDO-neglected	
	$U_{\mu\mu}$	$V_{\mu\nu,B}$	$\beta_{\mu\lambda}$	$U_{\mu\nu}$	$V_{\mu\lambda,C}$
CEP-4G	1072	54681	38112	2436	623544
STO-3G	1275	83130	53674	4060	878590
STO-6G	1275	83130	53674	4060	878590
3-21G	2347	272461	182252	15136	2982574
6-31G	2347	272461	182252	15136	2982574
6-311G	3188	502436	336336	30816	5065696
sum	11504	1268299	846300	71644	13411568

Table S2: The number of every type of *ab initio* 1-*e* integrals in different GTO basis sets for the Big Data analysis. The total number of 1-*e* integrals is approximately 15.6 million.

	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
$\bar{g}_{2\text{cx}}$	2.3	13.9	18.1	22.7	14.3	28.6
$\bar{g}_{3\text{cx}}$	0.0	2.7	16.5	27.6	22.9	30.3
$\bar{g}_{4\text{cx}}$	0.0	0.3	4.7	18.8	28.5	47.8

Table S3: Size distribution (in %) of *ab initio* 2-e exchange integrals in the Löwdin basis. The valence-only minimal CEP-4G basis function is employed for integral evaluation. The integrals are sorted into bins, from 10^{-1} to 10^{-6} eV, according to their exponent which is calculated in terms of $\text{floor}(\log_{10} |\bar{g}|)$ and $\text{floor}()$ is a Fortran intrinsic function. Exchange integrals with an absolute magnitude of less than 1.0×10^{-6} eV are counted into the 10^{-6} group.

		exchange integral			hybrid integral	
		$g_{2\text{cx}}$	$g_{3\text{cx}}$	$g_{4\text{cx}}$	$g_{2\text{ch}}$	$g_{3\text{ch}}$
STO-3G						
$\{\phi_i\}$	g_-	-4.516	-3.051	-1.566	-10.995	-4.582
	g_+	+5.227	+3.385	+1.823	+10.709	+5.384
$\{\bar{\phi}_\mu\}$	\bar{g}_-	-0.199	-0.201	-0.059	-3.031	-1.055
	\bar{g}_+	+0.683	+0.202	+0.046	+3.046	+1.055
STO-6G						
$\{\phi_i\}$	g_-	-4.516	-3.043	-1.567	-10.994	-4.564
	g_+	+5.226	+3.390	+1.826	+10.710	+5.389
$\{\bar{\phi}_\mu\}$	\bar{g}_-	-0.196	-0.190	-0.060	-3.042	-1.045
	\bar{g}_+	+0.654	+0.191	+0.045	+3.058	+1.045
3-21G						
$\{\phi_i\}$	g_-	-5.575	-5.341	-3.091	-14.952	-7.431
	g_+	+7.649	+5.432	+3.374	+14.632	+7.552
$\{\bar{\phi}_\mu\}$	\bar{g}_-	-0.519	-0.412	-0.258	-3.042	-2.366
	\bar{g}_+	+1.090	+0.464	+0.263	+3.001	+2.356
6-31G						
$\{\phi_i\}$	g_-	-5.923	-5.618	-3.389	-14.577	-7.847
	g_+	+7.568	+5.888	+3.725	+13.947	+7.932
$\{\bar{\phi}_\mu\}$	\bar{g}_-	-0.531	-0.432	-0.255	-3.422	-2.340
	\bar{g}_+	+1.084	+0.499	+0.263	+3.285	+2.329
6-311G						
$\{\phi_i\}$	g_-	-6.265	-5.557	-3.942	-14.665	-8.107
	g_+	+7.315	+5.803	+4.210	+14.503	+8.068
$\{\bar{\phi}_\mu\}$	\bar{g}_-	-0.529	-0.616	-0.271	-3.526	-1.680
	\bar{g}_+	+1.263	+0.650	+0.364	+3.496	+1.680

Table S4: The most negative values (g_- and \bar{g}_- , in eV) and the most positive values (g_+ and \bar{g}_+ , in eV) of the NDDO-neglected *ab initio* 2-e exchange and hybrid integrals in the atomic basis ($\{\phi_i\}$) and the Löwdin basis ($\{\bar{\phi}_\mu\}$), respectively. The following all-electron basis sets are employed for integral evaluation: single- ζ STO-3G and STO-6G, double- ζ 3-21G and 6-31G, and triple- ζ 6-311G.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+13.54	+12.35	-0.69	0.00	0.00	0.00	0.00
STO-3G	+29.04	+25.08	-0.32	0.00	0.00	0.00	0.00
STO-6G	+28.35	+25.27	-0.25	0.00	0.00	0.00	0.00
3-21G	+16.12	-63.48	-2.75	0.00	0.00	0.00	0.00
6-31G	-10.92	-64.71	-2.71	0.00	0.00	0.00	0.00
6-311G	+932.70	-71.69	-2.81	0.00	0.00	0.00	0.00

Table S5: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 1.

GTO	ΔE^{NDDO}	$\Delta E^{\bar{U}_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{\bar{V}_{\mu\lambda,\text{C}}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+28.15	+28.12	+4.65	+4.67	+14.65	-1.51	-0.20
STO-3G	+60.22	+50.05	+2.36	+2.65	+8.24	-0.89	-0.11
STO-6G	+60.55	+52.53	+2.40	+2.61	+8.16	-1.02	-0.11
3-21G	-3.01	-118.02	-10.47	-8.38	-18.74	-0.56	-0.10
6-31G	-33.33	-112.97	-9.75	-7.83	-18.23	-0.36	-0.09
6-311G	+963.70	-131.92	-14.05	-11.65	-27.04	-1.64	-0.23

Table S6: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 2.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+25.28	+24.66	+3.45	+3.61	+12.03	-1.14	-0.17
STO-3G	+53.57	+44.11	+3.05	+3.33	+9.48	-0.46	-0.10
STO-6G	+53.78	+46.34	+3.10	+3.30	+9.40	-0.55	-0.10
3-21G	-9.70	-107.05	-8.32	-5.62	-12.28	-0.04	-0.10
6-31G	-37.46	-102.49	-7.79	-5.28	-12.13	+0.13	-0.10
6-311G	+943.88	-122.12	-10.82	-7.49	-17.59	-0.50	-0.18

Table S7: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 3.

GTO	ΔE^{NDDO}	$\Delta E^{\bar{U}_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+26.53	+24.60	+0.61	+1.02	+6.48	-1.18	-0.05
STO-3G	+49.77	+41.26	+1.85	+2.19	+6.92	-0.38	-0.03
STO-6G	+50.29	+43.58	+1.98	+2.23	+6.93	-0.43	-0.04
3-21G	-12.07	-94.72	-7.12	-4.43	-7.67	-0.85	-0.03
6-31G	-36.53	-90.27	-6.39	-3.88	-6.71	-0.60	-0.01
6-311G	+924.75	-113.30	-7.93	-4.58	-9.51	-1.17	-0.01

Table S8: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 4.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+41.59	+41.53	+8.90	+8.69	+24.49	-2.23	-0.38
STO-3G	+90.23	+74.94	+4.20	+4.50	+13.21	-1.39	-0.23
STO-6G	+90.24	+78.18	+4.25	+4.41	+13.05	-1.56	-0.22
3-21G	-19.09	-184.93	-21.38	-18.59	-39.59	-1.09	-0.15
6-31G	-65.32	-177.77	-20.81	-18.28	-40.01	-0.89	-0.15
6-311G	+1423.36	-208.24	-28.69	-25.51	-56.77	-2.98	-0.47

Table S9: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 5.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+39.88	+39.32	+7.66	+7.58	+22.38	-2.04	-0.37
STO-3G	+86.00	+71.39	+5.84	+6.13	+16.56	-1.02	-0.23
STO-6G	+85.95	+74.46	+5.91	+6.06	+16.43	-1.15	-0.23
3-21G	-25.12	-172.44	-17.74	-14.36	-30.22	-0.41	-0.10
6-31G	-68.22	-165.47	-17.26	-14.17	-30.86	-0.23	-0.12
6-311G	+1403.90	-197.00	-23.27	-19.21	-43.12	-1.64	-0.33

Table S10: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 6.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+44.20	+42.71	+5.26	+5.46	+18.84	-2.41	-0.34
STO-3G	+86.45	+72.73	+6.67	+6.97	+18.25	-0.97	-0.20
STO-6G	+86.89	+76.10	+6.79	+6.96	+18.12	-1.07	-0.20
3-21G	-21.86	-154.03	-13.56	-10.50	-18.74	-0.56	+0.25
6-31G	-61.21	-147.23	-13.10	-10.26	-18.71	-0.35	+0.21
6-311G	+1392.34	-181.06	-17.46	-13.56	-28.40	-1.49	+0.17

Table S11: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 7.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+77.57	+76.48	+21.91	+21.07	+55.31	-4.37	-1.34
STO-3G	+176.23	+147.36	+19.95	+19.98	+48.62	-2.04	-0.85
STO-6G	+174.30	+151.61	+19.89	+19.63	+47.99	-2.22	-0.84
3-21G	-129.21	-374.09	-65.17	-58.85	-119.33	-2.81	-1.78
6-31G	-215.01	-361.95	-66.98	-61.34	-127.11	-2.84	-1.89
6-311G	+2681.38	-439.30	-84.67	-76.92	-166.50	-6.25	-3.03

Table S12: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 8.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+92.55	+91.54	+26.40	+25.33	+66.14	-5.21	-1.51
STO-3G	+208.80	+174.82	+23.07	+23.10	+56.28	-2.61	-1.00
STO-6G	+206.62	+179.90	+23.02	+22.72	+55.63	-2.83	-0.98
3-21G	-145.08	-440.20	-76.22	-69.42	-139.37	-2.42	-1.30
6-31G	-247.24	-426.55	-79.11	-73.07	-149.83	-2.59	-1.52
6-311G	+3139.32	-517.24	-101.06	-92.76	-198.86	-6.89	-2.73

Table S13: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 9.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+106.70	+105.67	+31.07	+29.76	+76.76	-5.98	-1.71
STO-3G	+239.24	+200.14	+25.17	+25.20	+61.73	-3.10	-1.10
STO-6G	+236.77	+205.99	+25.16	+24.81	+61.08	-3.36	-1.08
3-21G	-160.19	-506.55	-86.82	-79.45	-159.19	-2.57	-1.05
6-31G	-279.94	-492.03	-90.49	-83.96	-171.77	-2.79	-1.30
6-311G	+3598.16	-595.73	-117.39	-108.42	-231.78	-8.04	-2.71

Table S14: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 10.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+105.43	+103.98	+30.57	+29.39	+76.16	-5.82	-1.76
STO-3G	+236.72	+198.30	+28.26	+28.26	+68.04	-2.79	-1.18
STO-6G	+234.22	+204.01	+28.28	+27.90	+67.42	-3.02	-1.16
3-21G	-165.63	-492.45	-82.76	-74.75	-149.00	-2.04	-1.27
6-31G	-282.40	-478.33	-86.97	-79.86	-162.72	-2.32	-1.53
6-311G	+3580.43	-582.49	-112.42	-102.48	-219.23	-6.85	-2.86

Table S15: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 11.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+110.61	+108.38	+29.58	+28.69	+75.14	-6.18	-1.77
STO-3G	+239.00	+201.44	+30.88	+30.89	+73.22	-2.73	-1.15
STO-6G	+236.99	+207.48	+30.97	+30.60	+72.66	-2.92	-1.13
3-21G	-155.66	-467.48	-69.47	-61.84	-119.35	-0.95	+0.14
6-31G	-268.16	-453.69	-73.91	-67.08	-132.92	-1.22	-0.19
6-311G	+3576.84	-558.30	-95.64	-85.98	-180.44	-4.95	-0.78

Table S16: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 12.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+55.37	+54.16	+13.76	+12.64	+33.74	-2.35	-0.69
STO-3G	+128.26	+106.08	+11.55	+11.32	+28.39	-1.21	-0.45
STO-6G	+126.36	+108.87	+11.50	+11.06	+27.89	-1.35	-0.45
3-21G	-12.13	-294.00	-48.40	-44.42	-91.71	-2.40	-1.44
6-31G	-125.25	-289.74	-50.60	-46.98	-98.74	-2.78	-1.63
6-311G	+2819.41	-350.74	-62.62	-57.30	-124.91	-4.88	-2.35

Table S17: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 13.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+70.73	+69.76	+17.25	+15.89	+43.22	-3.29	-0.80
STO-3G	+161.83	+134.82	+14.73	+14.48	+36.37	-1.79	-0.57
STO-6G	+159.68	+138.46	+14.66	+14.16	+35.79	-1.98	-0.57
3-21G	-27.27	-359.90	-59.35	-54.87	-111.73	-2.10	-1.02
6-31G	-157.37	-354.62	-62.75	-58.67	-121.82	-2.57	-1.32
6-311G	+3278.87	-427.65	-78.16	-72.23	-155.79	-5.43	-2.09

Table S18: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 14.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+84.02	+82.94	+21.40	+19.80	+52.73	-4.03	-1.00
STO-3G	+191.94	+159.58	+16.49	+16.25	+41.13	-2.29	-0.69
STO-6G	+189.52	+164.02	+16.47	+15.94	+40.58	-2.51	-0.68
3-21G	-43.16	-426.50	-70.28	-65.19	-132.57	-2.45	-0.92
6-31G	-190.33	-420.11	-74.27	-69.67	-144.40	-2.91	-1.22
6-311G	+3737.49	-505.68	-94.28	-87.66	-188.46	-6.66	-2.17

Table S19: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 15.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+83.33	+81.89	+21.33	+19.86	+53.04	-3.87	-1.04
STO-3G	+189.89	+158.22	+19.81	+19.53	+47.93	-1.95	-0.73
STO-6G	+187.43	+162.51	+19.82	+19.24	+47.41	-2.13	-0.73
3-21G	-47.26	-411.41	-65.22	-59.54	-120.27	-1.84	-1.01
6-31G	-191.12	-405.07	-69.47	-64.32	-132.68	-2.33	-1.33
6-311G	+3721.86	-490.50	-87.22	-79.70	-171.45	-5.29	-2.16

Table S20: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 16.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+89.49	+87.49	+21.04	+19.86	+53.50	-4.17	-0.97
STO-3G	+192.99	+162.42	+23.02	+22.73	+54.37	-1.89	-0.70
STO-6G	+190.99	+167.01	+23.10	+22.50	+53.91	-2.04	-0.70
3-21G	-38.21	-387.46	-52.96	-47.76	-92.44	-1.18	+0.05
6-31G	-179.11	-382.69	-58.16	-53.34	-106.19	-1.66	-0.33
6-311G	+3715.99	-469.20	-73.36	-66.11	-138.44	-4.03	-0.61

Table S21: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 17.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+80.19	+80.08	+25.45	+24.20	+59.14	-4.27	-1.03
STO-3G	+180.50	+149.82	+11.72	+11.78	+31.14	-2.96	-0.64
STO-6G	+178.55	+154.27	+11.60	+11.40	+30.47	-3.18	-0.62
3-21G	-100.45	-405.36	-70.50	-66.23	-135.06	-3.34	-0.49
6-31G	-195.14	-392.05	-71.12	-67.42	-139.87	-3.25	-0.52
6-311G	+2754.52	-460.97	-92.55	-87.89	-187.84	-8.07	-1.56

Table S22: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 18.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+93.72	+93.58	+29.39	+27.91	+68.49	-4.99	-1.17
STO-3G	+209.79	+174.05	+12.81	+12.86	+34.58	-3.48	-0.77
STO-6G	+207.54	+179.26	+12.72	+12.46	+33.90	-3.74	-0.75
3-21G	-121.01	-477.00	-86.36	-81.49	-165.10	-3.68	-0.39
6-31G	-233.63	-463.05	-88.58	-84.38	-173.75	-3.74	-0.53
6-311G	+3206.63	-546.24	-115.97	-110.64	-234.91	-9.64	-1.85

Table S23: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 19.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+106.96	+106.81	+33.39	+31.69	+77.83	-5.72	-1.34
STO-3G	+239.33	+198.51	+14.13	+14.19	+38.52	-3.97	-0.86
STO-6G	+236.80	+204.49	+14.06	+13.78	+37.84	-4.27	-0.84
3-21G	-136.82	-544.26	-97.98	-92.40	-187.13	-3.98	-0.27
6-31G	-266.42	-529.14	-100.72	-95.91	-197.50	-4.07	-0.44
6-311G	+3664.72	-624.10	-132.09	-126.02	-267.71	-10.74	-1.91

Table S24: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 20.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+105.86	+105.19	+32.98	+31.40	+77.22	-5.50	-1.37
STO-3G	+236.15	+195.98	+16.92	+16.97	+44.10	-3.59	-0.88
STO-6G	+233.60	+201.84	+16.89	+16.59	+43.48	-3.86	-0.86
3-21G	-140.07	-528.41	-90.60	-84.41	-169.79	-2.84	+0.17
6-31G	-266.05	-512.96	-93.23	-87.84	-179.81	-2.96	0.00
6-311G	+3649.98	-608.51	-122.44	-115.42	-244.57	-8.87	-1.20

Table S25: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 21.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+111.58	+110.00	+32.34	+31.03	+77.00	-5.83	-1.38
STO-3G	+238.62	+199.32	+19.92	+20.00	+50.12	-3.52	-0.85
STO-6G	+236.56	+205.49	+19.98	+19.70	+49.54	-3.76	-0.83
3-21G	-131.36	-504.78	-81.10	-75.32	-147.59	-2.44	+0.96
6-31G	-254.90	-490.88	-84.91	-79.84	-159.49	-2.60	+0.70
6-311G	+3641.72	-588.81	-112.49	-105.66	-221.14	-8.04	-0.21

Table S26: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 22.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+59.51	+59.39	+17.59	+16.09	+40.23	-2.58	-0.49
STO-3G	+134.19	+111.84	+8.40	+8.11	+22.03	-1.85	-0.31
STO-6G	+132.22	+114.59	+8.28	+7.80	+21.54	-2.03	-0.30
3-21G	+9.64	-312.84	-54.07	-51.39	-105.25	-2.98	-0.85
6-31G	-110.57	-309.26	-55.34	-52.88	-110.40	-3.20	-0.92
6-311G	+2869.93	-363.76	-69.99	-66.49	-142.25	-6.48	-1.56

Table S27: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 23.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+72.99	+73.03	+21.06	+19.31	+48.90	-3.29	-0.61
STO-3G	+164.30	+136.99	+9.92	+9.62	+26.48	-2.35	-0.43
STO-6G	+162.02	+140.51	+9.80	+9.27	+25.92	-2.57	-0.42
3-21G	-8.79	-382.53	-67.58	-64.30	-130.95	-3.04	-0.59
6-31G	-147.07	-378.36	-70.15	-67.18	-139.34	-3.39	-0.77
6-311G	+3325.28	-445.48	-89.38	-85.25	-181.34	-7.47	-1.53

Table S28: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 24.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+86.14	+86.07	+24.95	+22.96	+57.99	-4.04	-0.80
STO-3G	+193.99	+161.44	+11.19	+10.89	+30.29	-2.86	-0.55
STO-6G	+191.44	+165.75	+11.11	+10.54	+29.75	-3.12	-0.54
3-21G	-25.91	-450.59	-79.71	-75.78	-154.06	-3.46	-0.53
6-31G	-181.73	-445.62	-83.19	-79.66	-164.80	-3.84	-0.72
6-311G	+3781.88	-525.71	-107.28	-102.40	-217.57	-8.79	-1.69

Table S29: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 25.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+85.25	+84.72	+24.83	+22.98	+57.95	-3.79	-0.80
STO-3G	+190.97	+159.16	+14.31	+14.01	+36.60	-2.47	-0.55
STO-6G	+188.40	+163.33	+14.27	+13.69	+36.11	-2.70	-0.54
3-21G	-27.67	-433.79	-71.89	-67.30	-135.89	-2.43	-0.22
6-31G	-179.37	-428.25	-75.00	-70.85	-145.86	-2.80	-0.40
6-311G	+3769.02	-507.31	-96.05	-90.23	-191.58	-6.92	-1.13

Table S30: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 26.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+89.36	+88.38	+23.18	+21.64	+55.84	-4.00	-0.77
STO-3G	+192.00	+161.48	+16.45	+16.19	+40.89	-2.38	-0.50
STO-6G	+189.89	+165.90	+16.45	+15.90	+40.39	-2.58	-0.49
3-21G	-22.91	-414.52	-66.56	-62.37	-122.52	-2.62	+0.15
6-31G	-171.22	-409.88	-69.94	-66.08	-132.19	-2.88	+0.03
6-311G	+3756.54	-491.50	-90.12	-84.57	-176.28	-6.57	-0.49

Table S31: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 27.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+63.87	+63.56	+5.96	+4.54	+17.92	-2.61	-0.38
STO-3G	+137.49	+116.16	+7.23	+6.73	+19.15	-1.50	-0.27
STO-6G	+136.48	+120.36	+7.68	+6.98	+19.79	-1.63	-0.27
3-21G	+137.71	-329.99	-38.48	-35.47	-72.37	-1.44	+0.15
6-31G	-55.15	-336.77	-47.26	-44.15	-92.34	-2.13	-0.16
6-311G	+4171.27	-402.47	-64.45	-59.98	-128.51	-4.80	-0.81

Table S32: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 28.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+89.40	+89.23	+12.92	+11.01	+34.46	-4.05	-0.72
STO-3G	+197.32	+166.03	+10.56	+10.04	+28.33	-2.54	-0.51
STO-6G	+195.70	+171.78	+11.09	+10.29	+29.03	-2.74	-0.50
3-21G	+101.30	-469.05	-66.14	-61.90	-125.16	-2.12	+0.36
6-31G	-129.33	-476.65	-79.48	-75.30	-155.54	-3.06	-0.18
6-311G	+5079.16	-570.06	-108.58	-102.70	-217.92	-7.76	-1.39

Table S33: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 29.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+87.45	+87.20	+17.91	+15.63	+42.64	-3.74	-0.68
STO-3G	+198.82	+167.64	+13.91	+13.14	+34.28	-2.49	-0.47
STO-6G	+196.08	+172.13	+14.20	+13.15	+34.48	-2.66	-0.47
3-21G	+82.13	-474.64	-71.31	-67.64	-137.44	-3.42	-0.31
6-31G	-148.26	-480.99	-82.53	-78.91	-163.95	-4.37	-0.74
6-311G	+5047.06	-571.45	-106.68	-101.45	-216.44	-8.68	-1.72

Table S34: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 30.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+121.22	+119.22	+22.58	+19.56	+55.64	-5.36	-1.23
STO-3G	+270.30	+227.81	+21.65	+20.51	+52.26	-3.04	-0.91
STO-6G	+266.60	+234.22	+22.24	+20.69	+52.80	-3.23	-0.90
3-21G	+92.79	-635.38	-88.13	-82.33	-165.16	-2.74	0.00
6-31G	-219.72	-644.30	-105.17	-99.59	-204.74	-4.12	-0.65
6-311G	+6882.11	-781.58	-141.25	-132.84	-282.16	-9.14	-1.94

Table S35: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 31.

GTO	ΔE^{NDDO}	$\Delta E^{U_{\mu\nu}}$	$\Delta E^{\bar{g}_{2\text{ch}}}$	$\Delta E^{\bar{g}_{2\text{cx}}}$	$\Delta E^{V_{\mu\lambda,C}}$	$\Delta E^{\bar{g}_{3\text{ch}}}$	$\Delta E^{\bar{g}_{3\text{cx}}}$
CEP-4G	+181.37	+179.59	+44.47	+40.57	+107.29	-9.21	-2.54
STO-3G	+406.47	+342.34	+42.75	+41.46	+100.90	-4.95	-1.79
STO-6G	+401.11	+351.56	+43.28	+41.37	+101.03	-5.25	-1.77
3-21G	-76.02	-920.34	-155.87	-146.41	-287.98	-2.54	+0.22
6-31G	-432.07	-923.18	-179.48	-170.88	-344.03	-4.50	-0.77

Table S36: Induced error (ΔE^i , in eV) relative to the standard HF-SCF electronic energy. See the text for the seven distinct schemes of neglecting *ab initio* molecular integrals. Gaussian-type orbital (GTO) basis functions are employed for integral evaluation. The serial number of the molecule in the test set is 32.

Mol.	CEP-4G	STO-3G	STO-6G	3-21G	6-31G	6-311G
1	-0.686	-0.319	-0.250	-2.750	-2.711	-2.807
2	-1.526	-1.187	-1.226	-2.642	-2.280	-4.031
3	-1.301	-0.746	-0.749	-2.748	-2.380	-3.830
4	-1.584	-0.726	-0.681	-3.538	-3.115	-4.525
5	-2.025	-1.692	-1.724	-3.875	-3.422	-6.158
6	-1.959	-1.302	-1.302	-3.786	-3.323	-5.708
7	-2.612	-1.277	-1.237	-3.617	-3.187	-5.382
8	-3.525	-2.069	-1.960	-9.129	-8.481	-13.998
9	-4.140	-2.640	-2.527	-9.217	-8.637	-15.193
10	-4.667	-3.134	-3.014	-9.942	-9.320	-17.005
11	-4.635	-2.792	-2.638	-10.042	-9.430	-16.789
12	-5.287	-2.749	-2.553	-8.574	-8.043	-14.603
13	-1.230	-0.977	-0.906	-6.389	-6.396	-10.199
14	-1.928	-1.548	-1.479	-6.579	-6.646	-11.353
15	-2.427	-2.049	-1.972	-7.540	-7.515	-13.282
16	-2.400	-1.670	-1.560	-7.518	-7.483	-12.810
17	-2.986	-1.598	-1.450	-6.377	-6.479	-11.278
18	-3.024	-3.012	-2.976	-7.606	-6.941	-12.731
19	-3.503	-3.526	-3.487	-8.551	-7.943	-14.971
20	-4.026	-4.033	-3.990	-9.551	-8.876	-16.810
21	-3.924	-3.642	-3.562	-9.033	-8.348	-15.894
22	-4.522	-3.604	-3.480	-8.224	-7.673	-14.870
23	-1.076	-1.560	-1.557	-5.666	-5.663	-9.977
24	-1.539	-2.048	-2.045	-6.320	-6.363	-11.600
25	-2.057	-2.561	-2.552	-7.386	-7.368	-13.670
26	-1.936	-2.160	-2.117	-7.022	-6.950	-12.744
27	-2.459	-2.115	-2.031	-6.810	-6.732	-12.120
28	-1.192	-1.003	-0.938	-4.453	-5.240	-9.264
29	-2.133	-2.012	-1.940	-6.357	-7.248	-13.640
30	-1.469	-1.717	-1.605	-7.097	-7.988	-13.903
31	-2.341	-1.901	-1.686	-8.532	-9.700	-17.548
32	-5.317	-3.657	-3.335	-11.994	-13.100	-

Table S37: Error (ΔE^{NAX} , in eV) relative to the HF-SCF molecular electronic energy calculated with the CEP-4G, STO-3G, STO-6G, 3-21G, 6-31G, and 6-311G basis functions. The NAX scheme is employed in the calculations. The NAX result for tryptophan in 6-311G is not available due to technical constraints.