

SUPPLEMENTARY MATERIAL

Component-wise AO Basis Reduction: Norm Loss, Negative Contribution Normalization, and Functional Implications

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Carbon. For the cc-pVTZ basis set ¹⁻³ normalization, carbon exhibits a reduction can be divided into two parts: predefined in system library of Gaussian 16 Rev. C.01 package and after reduction procedure in default calculations (Table S1).

Predefined system library has reduction. The reduction at $\alpha=0.9059$ and $\alpha=0.1285$ in the first block (AO labelled as S), which have contributions to the block 0.3399 % and 0.0048%, respectively, and causes a 4.1039 % and 0.0762 % loss in normalization. When considering the Join-block, the contributions change to 0.1834% and 0.0026%, while the corresponding normalizations loss change to 0.5524 % and 0.0371 %. Initially, the block consists of 9 primitives forming the constructive part $\phi_+(r)$, and 1 forming the destructive part $\phi_-(r)$. After predefined reduction, the block reduced to 7 constructive components.

Other reduced block is the third AO labelled as S at $\alpha=0.9059$ and $\alpha=0.1285$ also. However, the contribution is significant as their contribution to the block 3.9715% and 2.5854%, respectively, and causes 16.8646 % and 55.9772 % loss in normalization. When considering the Join-block, the contributions change to 1.9589 % and 6.0453 %, while the corresponding normalizations loss change to 0.6538% and 0.4256%. Initially, the block consists of 3 primitives forming the constructive part $\phi_+(r)$, and 7 forming the destructive part $\phi_-(r)$. After predefined reduction, the block reduced to 1 constructive component $\alpha=0.3643$.

The entire the fifth, ninth and twelfths, and fourteenth blocks AO labelled as S, P, D and F are reduced. The S block's $\alpha=0.04402$ by considering the Join-block, has contribution 0.4820 %, while the corresponding normalizations loss change to 11.2469%. The P block's $\alpha=0.0356$ by considering the Join-block, has contribution 0.4119 %, while the corresponding normalizations loss change to 10.3571%. The D block's $\alpha=0.1$ by considering the Join-block, has contribution 0.8919 %, while the corresponding normalizations loss change to 14.2150%. The F block's $\alpha=0.268$ by considering the Join-block, has contribution 1.8683%, while the corresponding normalizations loss change to 15.6563%.

Table S1. Norm loss and amplitude contribution per primitive Gaussian function for cc-pVTZ of C atom. The default reduction is labelled by stars (*) in system library.

A	$\phi^{(I)}$	α	$\delta_{loss}, \%$		$\delta_{contribution}, \%$	
			block	Join-block	block	Join-block
C	S	8236	0.0035	0.0000	4.2678	2.3026
		1235	0.0995	0.0010	7.9562	4.2926
		280.8	1.2503	0.0146	13.4473	7.2552
		79.27	8.8124	0.1237	20.2157	10.9069
		25.59	34.4174	0.6754	24.8374	13.4004
		8.997	65.8563	2.2053	20.9791	11.3188
		3.319	48.7229	2.9674	7.9126	4.2690
		0.9059*	4.1039	0.5524	0.3399	0.1834
		0.3643	-0.5872	-0.1457	0.0392	0.0211
		0.1285*	0.0762	0.0371	0.0048	0.0026
	S	0.9059	-	13.3284	-	4.6574
	S	8236	0.0002	-0.0000	2.9765	0.4900
		1235	0.0045	-0.0002	5.5729	0.9174
		280.8	0.0563	-0.0032	9.4883	1.5620
		79.27	0.3863	-0.0287	14.6769	2.4162
		25.59	1.286	-0.1722	19.3290	3.1821
		8.997	0.2664	-0.6961	20.0840	3.3064
		3.319	-8.4571	-1.5245	12.7625	2.1011
		0.9059*	16.8646	1.9589	3.9715	0.6538
		0.3643	75.3113	9.4443	8.5531	1.4081
		0.1285*	55.9772	6.0453	2.5854	0.4256
	S	0.1285	-	14.8493	-	1.0765
	S	0.04402*	-	11.2469	-	0.4820
	P	0.3827	-	15.4267	-	2.4405
	P	18.71	0.6314	0.0508	12.3152	0.6331
		4.133	8.3336	0.6871	24.5668	1.2629
		1.2	38.7535	3.7163	32.4643	1.6689
		0.3827*	69.2123	7.9110	23.7841	1.2227
		0.1209*	42.7612	5.2157	6.8695	0.3532
	P	0.1209	-	14.7101	-	1.0284
	P	0.03569*	-	10.3571	-	0.4119
	D	1.097	-	12.6332	-	5.3764
	D	0.318	-	15.5973	-	2.1240
	D	0.1*	-	14.2150	-	0.8919
	F	0.761	-	13.9027	-	4.0867
	F	0.268*	-	15.6563	-	1.8683

After reduction procedure. The reduction at $\alpha=0.3643$ in the first block (AO labelled as S), which have contributions to the block 0.0392 % and causes a -0.5872% loss in normalization (Negative meaning see in manuscript). When considering the Join-block, the contribution changes to 0.0211%, while the corresponding normalizations loss changes to -0.1457%. Initially, the block should consist consists of 9 primitives forming the constructive part $\phi_+(\mathbf{r})$, and 1 forming the destructive part $\phi_-(\mathbf{r})$. After all reductions, the block reduced to 7 constructive components only and destructive part $\phi_-(\mathbf{r})$ is reduced.

Other reduced block is the third AO labelled as S at $\alpha=8236$ and $\alpha=1235$ also. The contributions are to the block 2.9765% and 5.5729%, respectively, and causes 0.0002 % and 0.0045 % loss in normalization. When considering the Join-block, the contributions change to 0.4900% and 0.9174%, while the corresponding normalizations loss change to 0% and -0.0002%. Initially, the block consists of 3 primitives forming the constructive part $\phi_+(\mathbf{r})$, and 7 forming the destructive part $\phi_-(\mathbf{r})$. After predefined reduction, the block reduced to 1 constructive component and 5 destructive components.

References

- 1 B. P. Pritchard, D. Altarawy, B. Didier, T. D. Gibson, T. L. Windus, *J. Chem. Inf. Mod.* **2019**, 59, 4814-4820 10.1021/acs.jcim.9b00725.
- 2 T. H. Dunning, Jr., *J. Chem. Phys.* **1989**, 90, 1007-1023 10.1063/1.456153.
- 3 R. A. Kendall, T. H. Dunning, R. J. Harrison, *J. Chem. Phys.* **1992**, 96, 6796-6806 Doi 10.1063/1.462569.