Supporting Information to: Efficient Semi-Numerical Implementation of Relativistic Exact Exchange within the Infinite-Order Two-Component Method using a modified Chain-Of-Spheres Method

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1 Grid Parameters

1.1 General Grid Definition

Table 1: Definitions of Ahlrichs-type grids used in RAQET. n_{sphe} defines the number of spherical Gauss-Lebedev grid points for the inner, middle and outer atomic grid regions. The first and second value given for the middle region is used for hydrogen and all other elements, respectively. The number of radial mapped-Gauss-Chebychev grid points n_{rad} is given in terms of an element-specific offset.

		n_{sphe}		
Grid	inner	middle	outer	n_{rad}
0	26	50 - 50	50	n_{off}
1	26	50 - 50	110	n_{off}
2	26	$50 \ 50$	194	$n_{off}+5$
3	26	50 110	302	$n_{off} + 10$
4	26	$110 \ 110$	434	$n_{off} + 30$
5	26	$110 \ 110$	590	$n_{off} + 35$
6	26	110 110	974	$n_{off}+45$
7	26	$110 \ 110$	1202	$n_{off} + 65$
8	50	302 302	1454	$n_{off} + 160$

1.2 Other Parameters

For the elements of the different rows (with increasing order), the following offsets n_{off} have been used: 20 (H-He), 25 (Li-Ne), 35 (Na-Ar), 45 (K-Kr), 55 (Rb-Xe), 65 (Cs-Rn), 75 (Fr-Og). For the elements H, C, F, S, Cl, Br and I, the radial mapping parameters ξ have been re-optimized. The values 0.80, 1.16, 0.85, 0.95, 0.95, 0.92 and 0.97 have been used, respectively.

2 Scaling Comparison for Alkanethiols



Figure 1: Comparison of mCOSX computation times using the loose threshold set for the three levels of the PCT.

3 Parallel Efficiency of the mCOSX Method



Figure 2: Parallel efficiency of the mCOSX method and analytical integral evaluation for the H_2S molecule using the full PCT within the PCT density matrix scheme and the uncontracted cc-pVDZ basis set.