Evaluation of numerous J-, K-, L-, M-, and N-integrals used in perturbation theory: Integral raw data

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Following Pople and Gubbins & Gray, the *u*-expansion of the perturbation theory, used for developing equa-tions of state for fluids, requires sets of *J*-, *K*-, *L*-, *M*-, and *N*-integrals as a function of ρ^* and T^*. These integrals are calculated here from pair and triplet correlation functions, which were derived in a previous communication, using particle configurations from extensive *Monte-Carlo* simulations of a *Lennard-Jones* fluid. The pair and triplet correlation functions are based on 27615 state points covering a ρ^*-T^* space from 0.002 - 1.41 and 0.45 - 25 in reduced variables, respectively, which is also the range of the calculated integrals. Quadruplet correlation functions, required by the *M*- and *N*-integrals, were calculated using the *trans-superposition* approximation, using pair and triplet correlation functions. Here the unfitted raw data of 597 *J*-, 90 *K*-, 256 *L*-, 4 *M*-, and 4 *N*-integrals are reported. The number of available values at different ρ^*-T^* state points are 27615 for the *J*-integrals, and in the range of 6999 - 7053, 6789 -7055, 6440 - 6587, 6544 - 6751 for the *K*-, *L*-, *M*-, and *N*-integrals, respectively.

This technical report provides the integral raw data for numerous *J*-, *K*-, *L*-, *M*-, and *N*-integrals used in perturbation theory. The complete details of the nature, evaluation and resulting functions are given in Gottschalk[1]. Further information about the *Monte-Carlo* simulations and pair and triplet correlation functions are provided by Gottschalk[2–4].

Table I lists the available *J*-, *K*-, *L*-, *M*-, and *N*-integrals.

The data repository consist of the following compressed files: *J.zip*, *K.zip*, *L.zip*, *M.zip*, and *N.zip*. Each *zip* file includes all data files for each of the respective group of integrals (*J*-, *K*-, *L*-, *M*-, and *N*) as listed in Table I.

After unpacking, each individual integral file consists of rows of triplets (ρ^*, T^*, integral value). The number of data triplets are 27615 for the *J*-integrals and in the range of 6999 - 7053, 6789 - 7055, 6440 - 6587, 6544 - 6751 for the *K*-, *L*-, *M*-, and *N*-integrals, respectively.

The individual file name conventions are:

$J(n)).dat$,
$K((l,l',l''),(n,n',n'')).dat$,
$L(l,(n,n')).dat$,
$M((l,l',l''),(n,n',n'')).dat$, and
$N((l,l',l''),(n,n',n'')).dat$,

where l,l',l'',n,n',n'' are as listed as in Table I.

[1] M. Gottschalk, "Evaluation of numerous *J*-, *K*-, *L*-, *M*-, and *N*-integrals used in perturbation theory," Molecular Physics (2021), https://doi.org/10.1080/00268976.2021.2000652.

[2] M. Gottschalk, "An EOS for the Lennard-Jones fluid: A virial expansion approach," AIP Advances **9**, 125206 (2019), https://doi.org/10.1063/1.5119761.

[3] M. Gottschalk, "Calculation of pair and triplet correlation functions for a *Lennard-Jones* fluid at $\rho^* \leq 1.41$ and $t^* \leq 25$," AIP Advances **11**, 045026 (2021), https://doi.org/10.1063/5.0048450.

[4] M. Gottschalk, "Results of extensive *Monte Carlo* simulations for the *Lennard-Jones* fluid: Data for particle configurations, pair- and triplet-correlation functions in the range of $0.002 \leq \rho^* \leq 1.41$ and $0.45 \leq T^* \leq 25$," GFZ Data Services (2021), https://doi.org/10.5880/GFZ.3.6.2021.001.

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TABLE I. Quantity and type of calculated J, K, L, M, and N integrals.

J^n	$K^{n\,n'\,n''}_{l\,l'\,l''}$					$L^{n\,n'}_{l}$	$M^{n\,n'\,n''}_{l\,l'\,l''}$	$N^{n\,n'\,n''}_{l\,l'\,l''}$
597			90			256	4	4
$n: 4 \ldots 600 \in \mathbb{Z}$	$K^{3\,3\,3}_{2\,2\,2}$	$K^{12\,12\,12}_{2\,3\,3}$	$K^{12\,12\,12}_{2\,4\,4}$	$K^{12\,12\,6}_{3\,4\,5}$	$K^{12\,12\,7}_{4\,4\,6}$	$l: 1 \ldots 4 \in \mathbb{Z}$	$M^{12\,12\,12}_{2\,2\,2}$	$N^{12\,12\,12}_{2\,2\,2}$
	$K^{3\,3\,6}_{2\,2\,2}$	$K^{3\,5\,5}_{2\,4\,4}$	$K^{3\,6\,6}_{2\,5\,5}$	$K^{4\,6\,7}_{3\,5\,6}$	$K^{5\,6\,6}_{4\,5\,5}$	for $j,k: 4 \ldots 11 \in \mathbb{Z}$	$M^{12\,12\,12}_{2\,3\,3}$	$N^{12\,12\,12}_{2\,3\,3}$
	$K^{3\,3\,12}_{2\,2\,2}$	$K^{3\,5\,6}_{2\,4\,4}$	$K^{6\,6\,6}_{2\,5\,5}$	$K^{12\,6\,7}_{3\,5\,6}$	$K^{6\,6\,6}_{4\,5\,5}$	l odd:	$M^{12\,12\,12}_{3\,3\,4}$	$N^{12\,12\,12}_{3\,3\,4}$
	$K^{3\,6\,6}_{2\,2\,2}$	$K^{3\,5\,12}_{2\,4\,4}$	$K^{12\,6\,6}_{2\,5\,5}$	$K^{5\,5\,5}_{4\,4\,4}$	$K^{12\,6\,6}_{4\,5\,5}$	$n = 2j - 1$	$M^{12\,12\,12}_{4\,4\,4}$	$N^{12\,12\,12}_{4\,4\,4}$
	$K^{3\,6\,12}_{2\,2\,2}$	$K^{3\,6\,6}_{2\,4\,4}$	$K^{4\,4\,5}_{3\,3\,4}$	$K^{5\,5\,6}_{4\,4\,4}$	$K^{5\,6\,8}_{4\,5\,7}$	$n' = 2k - 1$		
	$K^{3\,12\,12}_{2\,2\,2}$	$K^{3\,6\,12}_{2\,4\,4}$	$K^{4\,4\,6}_{3\,3\,4}$	$K^{5\,5\,12}_{4\,4\,4}$	$K^{6\,6\,8}_{4\,5\,7}$	l even:		
	$K^{6\,6\,6}_{2\,2\,2}$	$K^{3\,12\,12}_{2\,4\,4}$	$K^{4\,4\,12}_{3\,3\,4}$	$K^{5\,6\,6}_{4\,4\,4}$	$K^{12\,6\,8}_{4\,5\,7}$	$n = 2j$		
	$K^{6\,6\,12}_{2\,2\,2}$	$K^{6\,5\,5}_{2\,4\,4}$	$K^{4\,12\,5}_{3\,3\,4}$	$K^{5\,6\,12}_{4\,4\,4}$	$K^{5\,7\,7}_{4\,6\,6}$	$n' = 2k$		
	$K^{6\,12\,12}_{2\,2\,2}$	$K^{6\,5\,6}_{2\,4\,4}$	$K^{4\,12\,6}_{3\,3\,4}$	$K^{5\,12\,12}_{4\,4\,4}$	$K^{6\,7\,7}_{4\,6\,6}$			
	$K^{12\,12\,12}_{2\,2\,2}$	$K^{6\,5\,12}_{2\,4\,4}$	$K^{4\,12\,12}_{3\,3\,4}$	$K^{6\,6\,6}_{4\,4\,4}$	$K^{12\,7\,7}_{4\,6\,6}$			
	$K^{3\,4\,4}_{2\,3\,3}$	$K^{6\,6\,6}_{2\,4\,4}$	$K^{12\,12\,5}_{3\,3\,4}$	$K^{6\,6\,12}_{4\,4\,4}$	$K^{6\,6\,7}_{5\,5\,6}$			
	$K^{3\,4\,12}_{2\,3\,3}$	$K^{6\,6\,12}_{2\,4\,4}$	$K^{12\,12\,6}_{3\,3\,4}$	$K^{6\,12\,12}_{4\,4\,4}$	$K^{6\,6\,9}_{5\,5\,8}$			
	$K^{3\,12\,12}_{2\,3\,3}$	$K^{6\,12\,12}_{2\,4\,4}$	$K^{12\,12\,12}_{3\,3\,4}$	$K^{12\,12\,12}_{4\,4\,4}$	$K^{6\,7\,8}_{5\,6\,7}$			
	$K^{6\,4\,4}_{2\,3\,3}$	$K^{12\,5\,5}_{2\,4\,4}$	$K^{4\,5\,6}_{3\,4\,5}$	$K^{5\,5\,7}_{4\,4\,6}$	$K^{7\,7\,7}_{6\,6\,6}$			
	$K^{6\,4\,12}_{2\,3\,3}$	$K^{12\,5\,6}_{2\,4\,4}$	$K^{4\,6\,6}_{3\,4\,5}$	$K^{5\,6\,7}_{4\,4\,6}$	$K^{7\,7\,9}_{6\,6\,8}$			
	$K^{6\,12\,12}_{2\,3\,3}$	$K^{12\,5\,12}_{2\,4\,4}$	$K^{4\,12\,6}_{3\,4\,5}$	$K^{5\,12\,7}_{4\,4\,6}$	$K^{7\,8\,8}_{6\,7\,7}$			
	$K^{12\,4\,4}_{2\,3\,3}$	$K^{12\,6\,6}_{2\,4\,4}$	$K^{12\,5\,6}_{3\,4\,5}$	$K^{6\,6\,7}_{4\,4\,6}$	$K^{8\,8\,9}_{7\,7\,8}$			
	$K^{12\,4\,12}_{2\,3\,3}$	$K^{12\,6\,12}_{2\,4\,4}$	$K^{12\,6\,6}_{3\,4\,5}$	$K^{6\,12\,7}_{4\,4\,6}$	$K^{9\,9\,9}_{8\,8\,8}$			