Electronic Supplementary Information to Exact quantum dynamics background of dispersion interactions: case study for CH_4·Ar in full (12) dimensions

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TABLE I. Normal coordinate parameters used in the present work for the methane fragment.

	q_1	q_2	q_3	q_4	q_5
ω^{har} [cm^{-1}]	3160.689	3160.689	3160.6892	3038.399	1571.950
Δx_{H_1}	0.0509759591	0.0546705578	0.0546705578	0.0572409089	−0.0562722869
Δy_{H_1}	0.0546705578	0.0509759591	0.0546705578	0.0572409089	−0.0562722869
Δz_{H_1}	0.0546705578	0.0546705578	0.0509759591	0.0572409089	0.1125445737
Δx_{H_2}	0.0509759591	0.0546705578	−0.0546705578	−0.0572409089	0.0562722869
Δy_{H_2}	0.0546705578	0.0509759591	−0.0546705578	−0.0572409089	0.0562722869
Δz_{H_2}	−0.0546705578	−0.0546705578	0.0509759591	0.0572409089	0.1125445737
Δx_{H_3}	0.0509759591	−0.0546705578	−0.0546705578	0.0572409089	−0.0562722869
Δy_{H_3}	−0.0546705578	0.0509759591	0.0546705578	−0.0572409089	0.0562722869
Δz_{H_3}	−0.0546705578	0.0546705578	0.0509759591	−0.0572409089	−0.1125445737
Δx_{H_4}	0.0509759591	−0.0546705578	0.0546705578	−0.0572409089	0.0562722869
Δy_{H_4}	−0.0546705578	0.0509759591	−0.0546705578	0.0572409089	−0.0562722869
Δz_{H_4}	0.0546705578	−0.0546705578	0.0509759591	−0.0572409089	−0.1125445737
Δx_{C}	−0.0171249492	0.0000000000	0.0000000000	0.0000000000	0.0000000000
Δy_{C}	0.0000000000	−0.0171249492	0.0000000000	0.0000000000	0.0000000000
Δz_{C}	0.0000000000	0.0000000000	−0.0171249492	0.0000000000	0.0000000000

	q_6	q_7	q_8	q_9	Reference	
ω^{har}	1571.950	1343.130	1343.130	1343.130	structure [bohr]:	
Δx_{H_1}	0.0974664599	0.1026140159	−0.0639110699	−0.0639110699	x_{H_1}	1.1935780397
Δy_{H_1}	−0.0974664599	−0.0639110699	0.1026140159	−0.0639110699	y_{H_1}	1.1935780397
Δz_{H_1}	0.0000000000	−0.0639110699	−0.0639110699	0.1026140159	z_{H_1}	1.1935780397
Δx_{H_2}	−0.0974664599	0.1026140159	−0.0639110699	0.0639110699	x_{H_2}	−1.1935780397
Δy_{H_2}	0.0974664599	−0.0639110699	0.1026140159	0.0639110699	y_{H_2}	−1.1935780397
Δz_{H_2}	0.0000000000	0.0639110699	0.0639110699	0.1026140159	z_{H_2}	1.1935780397
Δx_{H_3}	0.0974664599	0.1026140159	0.0639110699	0.0639110699	x_{H_3}	1.1935780397
Δy_{H_3}	0.0974664599	0.0639110699	0.1026140159	−0.0639110699	y_{H_3}	−1.1935780397
Δz_{H_3}	0.0000000000	0.0639110699	−0.0639110699	0.1026140159	z_{H_3}	−1.1935780397
Δx_{H_4}	−0.0974664599	0.1026140159	0.0639110699	−0.0639110699	x_{H_4}	−1.1935780397
Δy_{H_4}	−0.0974664599	0.0639110699	0.1026140159	0.0639110699	y_{H_4}	1.1935780397
Δz_{H_4}	0.0000000000	−0.0639110699	0.0639110699	0.1026140159	z_{H_4}	−1.1935780397
Δx_{C}	0.0000000000	−0.0344723247	0.0000000000	0.0000000000	x_{C}	0.0000000000
Δy_{C}	0.0000000000	0.0000000000	−0.0344723247	0.0000000000	y_{C}	0.0000000000
Δz_{C}	0.0000000000	0.0000000000	0.0000000000	−0.0344723247	z_{C}	0.0000000000