Supplementary Information: Accuracy of Diffusion Quantum Monte Carlo Method on Dissociation Curves of van der Waals Systems with Single-Slater-Jastrow Trial Wavefunction

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S1 Geometries of ten molecules at different inter-molecule distance(unit: Å)

CH4-F2 0.7

C	-0.099779142	-0.049213106	-0.049809806
H	-0.812383509	0.769437899	-0.053814782
H	-0.386626161	-0.773928179	0.705768112
H	0.890551861	0.333663823	0.175221084
H	-0.089826477	-0.524172039	-1.025860985
F	-0.827719852	-2.35344679	-0.471050203
F	-1.244272067	-3.668132309	-0.7047231

CH_4-F_2 0.8

C	-0.099779142	-0.049213106	-0.049809806
H	-0.812383509	0.769437899	-0.053814782
H	-0.386626161	-0.773928179	0.705768112
H	0.890551861	0.333663823	0.175221084
H	-0.089826477	-0.524172039	-1.025860985
F	-0.919288765	-2.643106031	-0.523678545
F	-1.335840980	-3.957791550	-0.757351442

CH_4-F_2 0.9

C	-0.099779142	-0.049213106	-0.049809806
H	-0.812383509	0.769437899	-0.053814782
H	-0.386626161	-0.773928179	0.705768112
H	0.890551861	0.333663823	0.175221084
H	-0.089826477	-0.524172039	-1.025860985
F	-1.010857678	-2.932765272	-0.576306887
F	-1.427409893	-4.247450791	-0.809979784

CH_4-F_2 1.0

C	-0.099779142	-0.049213106	-0.049809806
H	-0.812383509	0.769437899	-0.053814782
H	-0.386626161	-0.773928179	0.705768112
H	0.890551861	0.333663823	0.175221084
H	-0.089826477	-0.524172039	-1.025860985
F	-1.101049679	-3.218068940	-0.628143863
F	-1.517601894	-4.532754459	-0.861816760

CH_4-F_2 1.25

C	-0.099779142	-0.049213106	-0.049809806
H	-0.812383509	0.769437899	-0.053814782
H	-0.386626161	-0.773928179	0.705768112
H	0.890551861	0.333663823	0.175221084
H	-0.089826477	-0.524172039	-1.025860985

F -1.323042144 -3.920296008 -0.755731874
F -1.739594359 -5.234981527 -0.989404771
CH_4-F_2 1.5
C -0.099779142 -0.049213106 -0.049809806
H -0.812383509 0.769437899 -0.053814782
H -0.386626161 -0.773928179 0.705768112
H 0.890551861 0.333663823 0.175221084
H -0.089826477 -0.524172039 -1.025860985
F -1.542048797 -4.613078082 -0.881603819
F -1.958601012 -5.927763601 -1.115276716

CH_4-F_2 2.0
C -0.099779142 -0.049213106 -0.049809806
H -0.812383509 0.769437899 -0.053814782
H -0.386626161 -0.773928179 0.705768112
H 0.890551861 0.333663823 0.175221084
H -0.089826477 -0.524172039 -1.025860985
F -1.975788712 -5.985124242 -1.130891618
F -2.392340927 -7.299809761 -1.364564515

CH_4-Cl_2 0.7
C -0.029223000 -0.304334000 -0.044139000
Cl -1.583930727 -1.982155399 -0.718694605
Cl -2.886359727 -3.388877399 -1.283237605
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000
H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Cl_2 0.8
C -0.029223000 -0.304334000 -0.044139000
Cl -1.811091049 -2.227363603 -0.817226217
Cl -3.113520049 -3.634085603 -1.381769217
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000
H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Cl_2 0.9
C -0.029223000 -0.304334000 -0.044139000
Cl -2.038251371 -2.472571807 -0.915757829
Cl -3.340680371 -3.879293807 -1.480300829
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000

H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Cl_2 1.0

C -0.029223 -0.304334 -0.044139
Cl -2.261745 -2.713822 -1.012699
Cl -3.564174 -4.120544 -1.577242
H -1.013963 0.140625 -0.150390
H -0.061190 -1.086463 0.708351
H 0.678304 0.459656 0.262535
H 0.286077 -0.724543 -0.994403

CH_4-Cl_2 1.25

C -0.029223000 -0.304334000 -0.044139000
Cl -2.811142218 -3.306868814 -1.251002033
Cl -4.113571218 -4.713590814 -1.815545033
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000
H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Cl_2 1.5

C -0.029223000 -0.304334000 -0.044139000
Cl -3.352625156 -3.891372559 -1.485872218
Cl -4.655054156 -5.298094559 -2.050415218
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000
H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Cl_2 2.0

C -0.029223000 -0.304334000 -0.044139000
Cl -4.424274683 -5.048164617 -1.950704081
Cl -5.726703683 -6.454886617 -2.515247081
H -1.013963000 0.140625000 -0.150390000
H -0.061190000 -1.086463000 0.708351000
H 0.678304000 0.459656000 0.262535000
H 0.286077000 -0.724543000 -0.994403000

CH_4-Br_2 0.7

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329

H 0.274236028 -0.252091989 -1.050343280
Br -0.862479139 -2.145532273 -0.429940909
Br -1.723149959 -4.229681976 -0.80259836

CH_4-Br_2 0.8

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329
H 0.274236028 -0.252091989 -1.050343280
Br -0.994989432 -2.465309424 -0.487463977
Br -1.855660252 -4.549459127 -0.860121428

CH_4-Br_2 0.9

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329
H 0.274236028 -0.252091989 -1.050343280
Br -1.127499725 -2.785086575 -0.544987045
Br -1.988170545 -4.869236278 -0.917644496

CH_4-Br_2 1.0

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329
H 0.274236028 -0.252091989 -1.050343280
Br -1.257927165 -3.099837332 -0.601605941
Br -2.118597985 -5.183987035 -0.974263392

CH_4-Br_2 1.25

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329
H 0.274236028 -0.252091989 -1.050343280
Br -1.578688966 -3.873907725 -0.740849485
Br -2.439359786 -5.958057428 -1.113506936

CH_4-Br_2 1.5

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329

H 0.274236028 -0.252091989 -1.050343280
Br -1.894944789 -4.637104180 -0.878136972
Br -2.755615609 -6.721253883 -1.250794423

CH_4-Br_2 2.0

C 0.050957671 0.055164191 -0.032925885
H -1.024445640 0.072269161 0.117546172
H 0.508348983 -0.636912672 0.667869998
H 0.450713107 1.050360674 0.135265329
H 0.274236028 -0.252091989 -1.050343280
Br -2.521008076 -6.147935751 -1.149912697
Br -3.381678896 -8.232085454 -1.522570148

CH_4-I_2 0.7

C -0.032603000 -0.245329000 -0.035933000
I -1.735932251 -1.952081899 -0.874064591
I -3.510811251 -3.729086899 -1.746886591
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-I_2 0.8

C -0.032603000 -0.245329000 -0.035933000
I -1.981871883 -2.198447298 -0.995055871
I -3.756750883 -3.975452298 -1.867877871
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-I_2 0.9

C -0.032603000 -0.245329000 -0.035933000
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I -4.002690515 -4.221817697 -1.988869151
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-I_2 1.0

C -0.032603 -0.245329 -0.035933
I -2.470315 -2.687736 -1.235348
I -4.245194 -4.464741 -2.108170
H -0.980553 0.254481 -0.212468

H -0.160128 -1.020226 0.714308
H 0.692193 0.480189 0.320357
H 0.328323 -0.685520 -0.960895

CH_4-I_2 1.25

C -0.032603000 -0.245329000 -0.035933000
I -3.067794755 -3.286250102 -1.529281270
I -4.842673755 -5.063255102 -2.402103270
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-I_2 1.5

C -0.032603000 -0.245329000 -0.035933000
I -3.657769668 -3.877246369 -1.819522493
I -5.432648668 -5.654251369 -2.692344493
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-I_2 2.0

C -0.032603000 -0.245329000 -0.035933000
I -4.826941038 -5.048441789 -2.394702423
I -6.601820038 -6.825446789 -3.267524423
H -0.980553000 0.254481000 -0.212468000
H -0.160128000 -1.020226000 0.714308000
H 0.692193000 0.480189000 0.320357000
H 0.328323000 -0.685520000 -0.960895000

CH_4-CH_3F 0.7

C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C -0.150522693 0.086684027 -0.790648205
H -0.230892991 0.132119955 -1.872148117
H -1.009338302 -0.438284667 -0.384611934
H 0.760218551 -0.438926256 -0.519775671
H -0.124921141 1.093448258 -0.385984888

CH_4-CH_3F 0.8

C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C -0.083381747 0.048057171 -1.146937128
H -0.163752045 0.093493099 -2.228437040
H -0.942197356 -0.476911523 -0.740900857
H 0.827359497 -0.477553112 -0.876064594
H -0.057780195 1.054821402 -0.742273811

CH_4-CH_3F 0.9
C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C -0.016240801 0.009430315 -1.503226051
H -0.096611099 0.054866243 -2.584725963
H -0.875056410 -0.515538379 -1.097189780
H 0.894500443 -0.516179968 -1.232353517
H 0.009360751 1.016194546 -1.098562734

CH_4-CH_3F 1.0
C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C 0.047747496 -0.027382790 -1.842785183
H -0.032622802 0.018053138 -2.924285095
H -0.811068113 -0.552351484 -1.436748912
H 0.958488740 -0.552993073 -1.571912649
H 0.073349048 0.979381441 -1.438121866

CH_4-CH_3F 1.25
C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C 0.200245247 -0.115116267 -2.652026969
H 0.119874949 -0.069680339 -3.733526881
H -0.658570362 -0.640084961 -2.245990698

H 1.110986491 -0.640726550 -2.381154435
H 0.225846799 0.891647964 -2.247363652

CH_4-CH_3F 1.5
C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C 0.347002810 -0.199547357 -3.430807984
H 0.266632512 -0.154111429 -4.512307896
H -0.511812799 -0.724516051 -3.024771713
H 1.257744054 -0.725157640 -3.159935450
H 0.372604362 0.807216874 -3.026144667

CH_4-CH_3F 2.0
C 0.005918650 -0.003496527 1.853878993
F -1.172542855 0.674817567 1.614587488
H 0.830709843 0.546048289 1.407962789
H -0.056058041 -0.993747823 1.410355380
H 0.156078035 -0.088328739 2.927069055
C 0.632758458 -0.363945430 -4.947193697
H 0.552388160 -0.318509502 -6.028693609
H -0.226057151 -0.888914124 -4.541157426
H 1.543499702 -0.889555713 -4.676321163
H 0.658360010 0.642818801 -4.542530380

CH_4-CH_3Cl 0.7
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C -0.254210436 0.145592599 -0.733801631
H -0.326241469 0.177245695 -1.816426056
H -1.120601937 -0.367098082 -0.327833008
H 0.650694225 -0.383240624 -0.449706938
H -0.224412046 1.157892075 -0.343062947

CH_4-CH_3Cl 0.8
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712

H 0.311197296 -0.173143788 2.883203118
C -0.140609484 0.081366018 -1.110009988
H -0.212640517 0.113019114 -2.192634413
H -1.007000985 -0.431324663 -0.704041365
H 0.764295177 -0.447467205 -0.825915295
H -0.110811094 1.093665494 -0.719271304

CH_4-CH_3Cl 0.9
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C -0.027008532 0.017139437 -1.486218345
H -0.099039565 0.048792533 -2.568842770
H -0.893400033 -0.495551244 -1.080249722
H 0.877896129 -0.511693786 -1.202123652
H 0.002789858 1.029438913 -1.095479661

CH_4-CH_3Cl 1.0
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C 0.077602956 -0.042004770 -1.832656606
H 0.005571923 -0.010351674 -2.915281031
H -0.788788545 -0.554695451 -1.426687983
H 0.982507617 -0.570837993 -1.548561913
H 0.107401346 0.970294706 -1.441917922

CH_4-CH_3Cl 1.25
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C 0.320408328 -0.179279667 -2.636746790
H 0.248377295 -0.147626571 -3.719371215
H -0.545983173 -0.691970348 -2.230778167
H 1.225312989 -0.708112890 -2.352652097
H 0.350206718 0.833019809 -2.246008106

CH_4-CH_3Cl 1.5

C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C 0.549336098 -0.308708582 -3.394878996
H 0.477305065 -0.277055486 -4.477503421
H -0.317055403 -0.821399263 -2.988910373
H 1.454240759 -0.837541805 -3.110784303
H 0.579134488 0.703590894 -3.004140312

CH_4-CH_3Cl 2.0
C 0.052125307 -0.031919514 1.840660293
Cl -1.491715802 0.847207403 1.755184684
H 0.811909110 0.554725768 1.338264649
H -0.067811208 -0.989274688 1.347792712
H 0.311197296 -0.173143788 2.883203118
C 0.988909195 -0.557230067 -4.850598074
H 0.916878162 -0.525576971 -5.933222499
H 0.122517694 -1.069920748 -4.444629451
H 1.893813856 -1.086063290 -4.566503381
H 1.018707585 0.455069409 -4.459859390

CH_4-CHF_3 0.7
C 0.000023411 0.000105759 2.053285735
F -1.082526715 0.625339904 1.589816968
F 1.082627682 0.625237764 1.589922249
F -0.000023860 -1.249820225 1.589264753
H -0.000041960 -0.000280062 3.138092074
C -0.000001505 -5.867E-06 -0.88199114
H 0.000004947 0.000182705 -1.96751907
H -0.885649976 -0.511523877 -0.518711019
H 0.885736072 -0.51136885 -0.518700646
H -0.000092881 1.022627583 -0.518425109

CH_4-CHF_3 0.8
C 0.000023411 0.000105759 2.053285735
F -1.082526715 0.625339904 1.589816968
F 1.082627682 0.625237764 1.589922249
F -0.000023860 -1.249820225 1.589264753
H -0.000041960 -0.000280062 3.138092074
C -0.000005209 -0.000039061 -1.254630614
H 0.000001243 0.000149511 -2.340158544
H -0.885653680 -0.511557071 -0.891350493

H	0.885732368	-0.511402044	-0.891340120
H	-0.000096585	1.022594389	-0.891064583

CH_4-CHF_3 0.9

C	0.000023411	0.000105759	2.053285735
F	-1.082526715	0.625339904	1.589816968
F	1.082627682	0.625237764	1.589922249
F	-0.000023860	-1.249820225	1.589264753
H	-0.000041960	-0.000280062	3.138092074
C	-0.000008913	-0.000072255	-1.627270088
H	-0.000002461	0.000116317	-2.712798018
H	-0.885657384	-0.511590265	-1.263989967
H	0.885728664	-0.511435238	-1.263979594
H	-0.000100289	1.022561195	-1.263704057

CH_4-CHF_3 1.0

C	0.000023411	0.000105759	2.053285735
F	-1.082526715	0.625339904	1.589816968
F	1.082627682	0.625237764	1.589922249
F	-0.000023860	-1.249820225	1.589264753
H	-0.000041960	-0.000280062	3.138092074
C	-0.000012548	-0.000104834	-1.992998099
H	-0.000006096	0.000083738	-3.078526029
H	-0.885661019	-0.511622844	-1.629717978
H	0.885725029	-0.511467817	-1.629707605
H	-0.000103924	1.022528616	-1.629432068

CH_4-CHF_3 1.25

C	0.000023411	0.000105759	2.053285735
F	-1.082526715	0.625339904	1.589816968
F	1.082627682	0.625237764	1.589922249
F	-0.000023860	-1.249820225	1.589264753
H	-0.000041960	-0.000280062	3.138092074
C	-0.000021461	-0.000184713	-2.889721919
H	-0.000015009	0.000003859	-3.975249849
H	-0.885669932	-0.511702723	-2.526441798
H	0.885716116	-0.511547696	-2.526431425
H	-0.000112837	1.022448737	-2.526155888

CH_4-CHF_3 1.5

C	0.000023411	0.000105759	2.053285735
F	-1.082526715	0.625339904	1.589816968
F	1.082627682	0.625237764	1.589922249
F	-0.000023860	-1.249820225	1.589264753

H -0.000041960 -0.000280062 3.138092074
C -0.000030228 -0.000263279 -3.771712327
H -0.000023776 -0.000074707 -4.857240257
H -0.885678699 -0.511781289 -3.408432206
H 0.885707349 -0.511626262 -3.408421833
H -0.000121604 1.022370171 -3.408146296

CH_4-CHF_3 2.0
C 0.000023411 0.000105759 2.053285735
F -1.082526715 0.625339904 1.589816968
F 1.082627682 0.625237764 1.589922249
F -0.000023860 -1.249820225 1.589264753
H -0.000041960 -0.000280062 3.138092074
C -0.000047553 -0.000418544 -5.514713708
H -0.000041101 -0.000229972 -6.600241638
H -0.885696024 -0.511936554 -5.151433587
H 0.885690024 -0.511781527 -5.151423214
H -0.000138929 1.022214906 -5.151147677

CH_4-$CHCl_3$ 0.7
C -0.000028509 -0.000461929 2.158149022
Cl -1.454063734 0.838777303 1.616235012
Cl 1.454144531 0.838659727 1.616208515
Cl -0.000087400 -1.679795034 1.617802938
H 0.000005696 0.000267325 3.239305949
C -0.000020378 0.000101581 -0.829012152
H 0.00002731 -0.00176743 -1.914768206
H -0.88549756 -0.510632424 -0.463880631
H 0.88562606 -0.510482141 -0.463844203
H -0.000090521 1.023277977 -0.466499953

CH_4-$CHCl_3$ 0.8
C -0.000028509 -0.000461929 2.158149022
Cl -1.454063734 0.838777303 1.616235012
Cl 1.454144531 0.838659727 1.616208515
Cl -0.000087400 -1.679795034 1.617802938
H 0.000005696 0.000267325 3.239305949
C -0.000021421 0.000239906 -1.240255582
H 0.000026267 -0.001629105 -2.326011636
H -0.885498603 -0.510494099 -0.875124061
H 0.885625017 -0.510343816 -0.875087633
H -0.000091564 1.023416302 -0.877743383

CH_4-$CHCl_3$ 0.9

C	-0.000028509	-0.000461929	2.158149022
Cl	-1.454063734	0.838777303	1.616235012
Cl	1.454144531	0.838659727	1.616208515
Cl	-0.000087400	-1.679795034	1.617802938
H	0.000005696	0.000267325	3.239305949
C	-0.000022464	0.000378231	-1.651499012
H	0.000025224	-0.001490780	-2.737255066
H	-0.885499646	-0.510355774	-1.286367491
H	0.885623974	-0.510205491	-1.286331063
H	-0.000092607	1.023554627	-1.288986813

CH_4-$CHCl_3$ 1.0

C	-0.000028509	-0.000461929	2.158149022
Cl	-1.454063734	0.838777303	1.616235012
Cl	1.454144531	0.838659727	1.616208515
Cl	-0.000087400	-1.679795034	1.617802938
H	0.000005696	0.000267325	3.239305949
C	-0.000023477	0.000512590	-2.050951410
H	0.000024211	-0.001356421	-3.136707464
H	-0.885500659	-0.510221415	-1.685819889
H	0.885622961	-0.510071132	-1.685783461
H	-0.000093620	1.023688986	-1.688439211

CH_4-$CHCl_3$ 1.25

C	-0.000028509	-0.000461929	2.158149022
Cl	-1.454063734	0.838777303	1.616235012
Cl	1.454144531	0.838659727	1.616208515
Cl	-0.000087400	-1.679795034	1.617802938
H	0.000005696	0.000267325	3.239305949
C	-0.000025935	0.000838583	-3.020135282
H	0.000021753	-0.001030428	-4.105891336
H	-0.885503117	-0.509895422	-2.655003761
H	0.885620503	-0.509745139	-2.654967333
H	-0.000096078	1.024014979	-2.657623083

CH_4-$CHCl_3$ 1.5

C	-0.000028509	-0.000461929	2.158149022
Cl	-1.454063734	0.838777303	1.616235012
Cl	1.454144531	0.838659727	1.616208515
Cl	-0.000087400	-1.679795034	1.617802938
H	0.000005696	0.000267325	3.239305949
C	-0.000028332	0.001156578	-3.965541535
H	0.000019356	-0.000712433	-5.051297589
H	-0.885505514	-0.509577427	-3.600410014

H 0.885618106 -0.509427144 -3.600373586
H -0.000098475 1.024332974 -3.603029336

CH_4-$CHCl_3$ 2.0
C -0.000028509 -0.000461929 2.158149022
Cl -1.454063734 0.838777303 1.616235012
Cl 1.454144531 0.838659727 1.616208515
Cl -0.000087400 -1.679795034 1.617802938
H 0.000005696 0.000267325 3.239305949
C -0.000033043 0.001781404 -5.823159317
H 0.000014645 -0.000087607 -6.908915371
H -0.885510225 -0.508952601 -5.458027796
H 0.885613395 -0.508802318 -5.457991368
H -0.000103186 1.024957800 -5.460647118

CH_3F-CH_3F 0.7
C 0.250211388 -0.141261283 2.278305952
F 0.055015573 -0.060688554 0.911538424
H 1.189310250 0.342978795 2.531275149
H 0.282891774 -1.187166859 2.570525524
H -0.571443596 0.358513497 2.783864006
C -0.139515065 0.072084244 -1.211198078
F -0.270371254 0.175266689 -2.58454131
H -0.990708073 -0.470513541 -0.810432282
H 0.777569057 -0.46114603 -0.978318201
H -0.103714934 1.067817603 -0.779120993

CH_3F-CH_3F 0.8
C 0.250211388 -0.141261283 2.278305952
F 0.055015573 -0.060688554 0.911538424
H 1.189310250 0.342978795 2.531275149
H 0.282891774 -1.187166859 2.570525524
H -0.571443596 0.358513497 2.783864006
C -0.171682962 0.092497084 -1.527470165
F -0.302539151 0.195679529 -2.900813397
H -1.022875970 -0.450100701 -1.126704369
H 0.745401160 -0.440733190 -1.294590288
H -0.135882831 1.088230443 -1.095393080

CH_3F-CH_3F 0.9
C 0.250211388 -0.141261283 2.278305952
F 0.055015573 -0.060688554 0.911538424
H 1.189310250 0.342978795 2.531275149
H 0.282891774 -1.187166859 2.570525524

H	-0.571443596	0.358513497	2.783864006
C	-0.203850859	0.112909924	-1.843742252
F	-0.334707048	0.216092369	-3.217085484
H	-1.055043867	-0.429687861	-1.442976456
H	0.713233263	-0.420320350	-1.610862375
H	-0.168050728	1.108643283	-1.411665167

CH_3F-CH_3F 1.0

C	0.250211388	-0.141261283	2.278305952
F	0.055015573	-0.060688554	0.911538424
H	1.189310250	0.342978795	2.531275149
H	0.282891774	-1.187166859	2.570525524
H	-0.571443596	0.358513497	2.783864006
C	-0.235364089	0.132907332	-2.153577716
F	-0.366220278	0.236089777	-3.526920948
H	-1.086557097	-0.409690453	-1.752811920
H	0.681720033	-0.400322942	-1.920697839
H	-0.199563958	1.128640691	-1.721500631

CH_3F-CH_3F 1.25

C	0.250211388	-0.141261283	2.278305952
F	0.055015573	-0.060688554	0.911538424
H	1.189310250	0.342978795	2.531275149
H	0.282891774	-1.187166859	2.570525524
H	-0.571443596	0.358513497	2.783864006
C	-0.312494045	0.181851828	-2.911913043
F	-0.443350234	0.285034273	-4.285256275
H	-1.163687053	-0.360745957	-2.511147247
H	0.604590077	-0.351378446	-2.679033166
H	-0.276693914	1.177585187	-2.479835958

CH_3F-CH_3F 1.5

C	0.250211388	-0.141261283	2.278305952
F	0.055015573	-0.060688554	0.911538424
H	1.189310250	0.342978795	2.531275149
H	0.282891774	-1.187166859	2.570525524
H	-0.571443596	0.358513497	2.783864006
C	-0.388243394	0.229920230	-3.656674352
F	-0.519099583	0.333102675	-5.030017584
H	-1.239436402	-0.312677555	-3.255908556
H	0.528840728	-0.303310044	-3.423794475
H	-0.352443263	1.225653589	-3.224597267

CH_3F-CH_3F 2.0

C 0.250211388 -0.141261283 2.278305952
F 0.055015573 -0.060688554 0.911538424
H 1.189310250 0.342978795 2.531275149
H 0.282891774 -1.187166859 2.570525524
H -0.571443596 0.358513497 2.783864006
C -0.537785093 0.324815177 -5.126955922
F -0.668641282 0.427997622 -6.500299154
H -1.388978101 -0.217782608 -4.726190126
H 0.379299029 -0.208415097 -4.894076045
H -0.501984962 1.320548536 -4.694878837

CH_3Cl-CH_3Cl 0.7
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.167178835 0.086892488 -1.431079387
Cl -0.349835401 0.206306254 -3.197592322
H -1.016179191 -0.454796092 -1.031499545
H 0.75261494 -0.442221946 -1.212821816
H -0.131752165 1.087868141 -1.018190727

CH_3Cl-CH_3Cl 0.8
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.197707281 0.109748582 -1.778991069
Cl -0.380363847 0.229162348 -3.545504004
H -1.046707637 -0.431939998 -1.379411227
H 0.722086494 -0.419365852 -1.560733498
H -0.162280611 1.110724235 -1.366102409

CH_3Cl-CH_3Cl 0.9
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.228235727 0.132604676 -2.126902751
Cl -0.410892293 0.252018442 -3.893415686
H -1.077236083 -0.409083904 -1.727322909

H 0.691558048 -0.396509758 -1.908645180
H -0.192809057 1.133580329 -1.714014091

CH_3Cl-CH_3Cl 1.0
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.258353838 0.155153560 -2.470138140
Cl -0.441010404 0.274567326 -4.236651075
H -1.107354194 -0.386535020 -2.070558298
H 0.661439937 -0.373960874 -2.251880569
H -0.222927168 1.156129213 -2.057249480

CH_3Cl-CH_3Cl 1.25
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.332603474 0.210742916 -3.316310144
Cl -0.515260040 0.330156682 -5.082823079
H -1.181603830 -0.330945664 -2.916730302
H 0.587190301 -0.318371518 -3.098052573
H -0.297176804 1.211718569 -2.903421484

CH_3Cl-CH_3Cl 1.5
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143
H -0.501709016 0.328185531 3.291345152
C -0.405954921 0.265659815 -4.152246112
Cl -0.588611487 0.385073581 -5.918759047
H -1.254955277 -0.276028765 -3.752666270
H 0.513838854 -0.263454619 -3.933988541
H -0.370528251 1.266635468 -3.739357452

CH_3Cl-CH_3Cl 2.0
C 0.301152114 -0.173118099 2.764480435
Cl -0.024870834 -0.077582132 1.017161127
H 1.247502252 0.314602623 2.964654708
H 0.346131151 -1.217442126 3.048836143

```
H   -0.501709016   0.328185531   3.291345152
C   -0.551367228   0.374527373  -5.809410101
Cl   -0.734023794   0.493941139  -7.575923036
H   -1.400367584  -0.167161207  -5.409830259
H    0.368426547  -0.154587061  -5.591152530
H   -0.515940558   1.375503026  -5.396521441
```

S2 Total energies of ten molecules at different inter-molecule distance by CCSD(T)-PP/aug-cc-pVTZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.457233	-56.462558	-56.463595	-56.463501	-56.462903	-56.462635	-56.462475
CH_4-Cl2	-37.932635	-37.950927	-37.955075	-37.955335	-37.954111	-37.953533	-37.953242
CH_4-Br_2	-34.695192	-34.717478	-34.722899	-34.723416	-34.722067	-34.721419	-34.721089
CH_4-I_2	-30.832037	-30.856076	-30.861779	-30.862220	-30.860590	-30.859857	-30.859506
CH_3F-CH_3F	-63.466916	-63.482055	-63.485297	-63.485411	-63.484249	-63.483602	-63.483095
CH_3Cl-CH_3Cl	-44.840328	-44.856718	-44.860427	-44.860683	-44.859588	-44.858980	-44.858596
CH_3F-CH_4	-39.803573	-39.814673	-39.816857	-39.816845	-39.816065	-39.815734	-39.815562
CH_3Cl-CH_4	-30.482110	-30.501067	-30.504959	-30.505109	-30.504107	-30.503642	-30.503396
CHF_3-CH_4	-87.192938	-87.201309	-87.202613	-87.202370	-87.201536	-87.201243	-87.201099
$CHCl_3$-CH_4	-59.191482	-59.208779	-59.212568	-59.212620	-59.211310	-59.210764	-59.210498

S3 Total energies of ten molecules at different inter-molecule distance by CCSD(T)-PP/aug-cc-pVQZ. (unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.505165	-56.510497	-56.511583	-56.511551	-56.511050	-56.510836	-56.510727
CH_4-Cl2	-37.983641	-38.001427	-38.005387	-38.005609	-38.004497	-38.004015	-38.003792
CH_4-Br_2	-34.753135	-34.774966	-34.780150	-34.780576	-34.779233	-34.778620	-34.778345
CH_4-I_2	-30.899444	-30.923203	-30.928944	-30.929485	-30.928090	-30.927451	-30.927168
CH_3F-CH_3F	-63.523964	-63.539072	-63.542339	-63.542478	-63.541357	-63.540729	-63.540254
CH_3Cl-CH_3Cl	-44.898316	-44.914383	-44.917980	-44.918212	-44.917165	-44.916631	-44.916276
CH_3F-CH_4	-39.840367	-39.851448	-39.853686	-39.853724	-39.853010	-39.852699	-39.852546
CH_3Cl-CH_4	-30.519149	-30.538056	-30.542008	-30.542223	-30.541295	-30.540865	-30.540646
CHF_3-CH_4	-87.269929	-87.278436	-87.279903	-87.279750	-87.279035	-87.278776	-87.278662
$CHCl_3$-CH_4	-59.269138	-59.286483	-59.290467	-59.290668	-59.289473	-59.288965	-59.288739

S4 Total energies of ten molecules at different inter-molecule distance by CCSD-PP/aug-cc-pVTZ. (unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.430356	-56.436144	-56.437420	-56.437453	-56.436976	-56.436740	-56.436596
CH_4-Cl2	-37.903662	-37.922867	-37.927516	-37.928052	-37.927103	-37.926599	-37.926340
CH_4-Br_2	-34.671241	-34.694497	-34.700465	-34.701293	-34.700263	-34.699699	-34.699408
CH_4-I_2	-30.809269	-30.834271	-30.840554	-30.841334	-30.840064	-30.839427	-30.839118
CH_3F-CH_3F	-63.437443	-63.452985	-63.456464	-63.456711	-63.455677	-63.455060	-63.454561
CH_3Cl-CH_3Cl	-44.804713	-44.821870	-44.826008	-44.826504	-44.825651	-44.825109	-44.824753
CH_3F-CH_4	-39.781732	-39.793303	-39.795769	-39.795916	-39.795296	-39.795008	-39.794855
CH_3Cl-CH_4	-30.457020	-30.476714	-30.481033	-30.481414	-30.480641	-30.480241	-30.480024
CHF_3-CH_4	-87.154671	-87.163466	-87.165030	-87.164938	-87.164257	-87.164002	-87.163876
$CHCl_3$-CH_4	-59.142183	-59.160448	-59.164809	-59.165186	-59.164202	-59.163741	-59.163513

S5 Total energies of ten molecules at different inter-molecule distance by CCSD-PP/aug-cc-pVQZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.475959	-56.481766	-56.483094	-56.483189	-56.482810	-56.482628	-56.482533
CH_4-Cl2	-37.950560	-37.969324	-37.973815	-37.974327	-37.973493	-37.973080	-37.972887
CH_4-Br_2	-34.725262	-34.748117	-34.753890	-34.754649	-34.753643	-34.753116	-34.752876
CH_4-I_2	-30.871771	-30.896533	-30.902877	-30.903769	-30.902734	-30.902188	-30.901942
CH_3F-CH_3F	-63.491898	-63.507422	-63.510931	-63.511207	-63.510220	-63.509622	-63.509154
CH_3Cl-CH_3Cl	-44.858345	-44.875234	-44.879287	-44.879772	-44.878975	-44.878503	-44.878175
CH_3F-CH_4	-39.816789	-39.828360	-39.830885	-39.831083	-39.830531	-39.830263	-39.830130
CH_3Cl-CH_4	-30.491448	-30.511126	-30.515519	-30.515968	-30.515274	-30.514908	-30.514718
CHF_3-CH_4	-87.228214	-87.237154	-87.238882	-87.238879	-87.238315	-87.238095	-87.237998
$CHCl_3$-CH_4	-59.213646	-59.232006	-59.236580	-59.237112	-59.236247	-59.235826	-59.235636

S6 Total energies of ten molecules at different inter-molecule distance by MP2-PP/aug-cc-pVTZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.404164	-56.409122	-56.410018	-56.409873	-56.409243	-56.408969	-56.408807
CH_4-Cl2	-37.854400	-37.871435	-37.875035	-37.875057	-37.873650	-37.873028	-37.872713
CH_4-Br_2	-34.628427	-34.649346	-34.654124	-34.654353	-34.652777	-34.652075	-34.651718
CH_4-I_2	-30.767789	-30.790614	-30.795708	-30.795870	-30.794019	-30.793231	-30.792853
CH_3F-CH_3F	-63.401685	-63.416729	-63.420024	-63.420206	-63.419136	-63.418515	-63.418020
CH_3Cl-CH_3Cl	-44.745537	-44.761100	-44.764461	-44.764571	-44.763369	-44.762735	-44.762333
CH_3F-CH_4	-39.743815	-39.754879	-39.757108	-39.757142	-39.756420	-39.756104	-39.755936
CH_3Cl-CH_4	-30.407636	-30.426115	-30.429838	-30.429936	-30.428909	-30.428439	-30.428186
CHF_3-CH_4	-87.123627	-87.132105	-87.133528	-87.133366	-87.132614	-87.132339	-87.132202
$CHCl_3$-CH_4	-59.079209	-59.095616	-59.099006	-59.098886	-59.097447	-59.096868	-59.096583

S7 Total energies of ten molecules at different inter-molecule distance by MP2-PP/aug-cc-pVQZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.456412	-56.461368	-56.462302	-56.462208	-56.461659	-56.461432	-56.461317
CH_4-Cl2	-37.906982	-37.923497	-37.926893	-37.926871	-37.925568	-37.925038	-37.924792
CH_4-Br_2	-34.687865	-34.708289	-34.712808	-34.712928	-34.711335	-34.710657	-34.710351
CH_4-I_2	-30.834271	-30.856736	-30.861816	-30.862040	-30.860371	-30.859661	-30.859342
CH_3F-CH_3F	-63.464311	-63.479313	-63.482622	-63.482822	-63.481787	-63.481184	-63.480719
CH_3Cl-CH_3Cl	-44.806760	-44.821972	-44.825208	-44.825288	-44.824116	-44.823545	-44.823169
CH_3F-CH_4	-39.785545	-39.796570	-39.798839	-39.798916	-39.798248	-39.797947	-39.797797
CH_3Cl-CH_4	-30.448500	-30.466867	-30.470619	-30.470768	-30.469796	-30.469352	-30.469122
CHF_3-CH_4	-87.206755	-87.215348	-87.216916	-87.216830	-87.216182	-87.215936	-87.215825
$CHCl_3$-CH_4	-59.159825	-59.176183	-59.179717	-59.179718	-59.178358	-59.177807	-59.177557

S8 Total energies and error bars of ten molecules at different inter-molecule distance by DMC-Tmoves/aug-cc-pVTZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.491448/ 0.000104	-56.496927/ 0.000105	-56.498157/ 0.000095	-56.498239/ 0.000102	-56.497528/ 0.0001	-56.497488/ 0.000095	-56.497457/ 0.000094
CH_4-Cl_2	-37.987598/ 0.000095	-38.005422/ 0.000096	-38.00977/ 0.000099	-38.00957/ 0.000105	-38.008951/ 0.000099	-38.009299/ 0.000088	-38.009183/ 0.000087
CH_4-Br_2	-34.763236/ 0.0001	-34.78625/ 0.000091	-34.791827/ 0.000091	-34.791995/ 0.000089	-34.791197/ 0.00008	-34.790591/ 0.000083	-34.790244/ 0.000086
CH_4-I_2	-30.907227/ 0.000085	-30.926036/ 0.000128	-30.937568/ 0.000082	-30.938035/ 0.000084	-30.936613/ 0.000079	-30.936581/ 0.000082	-30.933286/ 0.000103
CH_3F-CH_3F	-63.517265/ 0.000116	-63.532594/ 0.000106	-63.536251/ 0.000114	-63.536469/ 0.000103	63.535492/ 0.000109	-63.534647/ 0.000105	-63.534068/ 0.000108
CH_3Cl-CH_3Cl	-44.900619/ 0.000115	-44.91647/ 0.000117	-44.919241/ 0.000132	-44.920952/ 0.000112	-44.920348/ 0.000107	-44.919418/ 0.000116	-44.919286/ 0.000110
CH_3F-CH_4	-39.835052/ 0.000096	-39.846974/ 0.000095	-39.849135/ 0.000093	-39.849324/ 0.000093	-39.848662/ 0.000091	-39.848488/ 0.000088	-39.848083/ 0.000083
CH_3Cl-CH_4	-30.518108 0.000099	-30.537797/ 0.000088	-30.541565/ 0.000094	-30.542149/ 0.000095	-30.541488/ 0.000091	-30.541323/ 0.000085	-30.540927/ 0.000084
CHF_3-CH_4	-87.263018/ 0.000119	-87.271659/ 0.000115	-87.273228/ 0.000113	-87.273198/ 0.00012	-87.273095/ 0.000113	-87.272216/ 0.000115	-87.271985/ 0.000117
$CHCl_3$-CH_4	-59.272004/ 0.000127	-59.289301/ 0.000132	-59.294254/ 0.000131	-59.294649/ 0.00012	-59.294053/ 0.000118	-59.292995/ 0.000127	-59.293127/ 0.000124

S9 Total energies and error bars of ten molecules at different inter-molecule distance by DMC-DLA/aug-cc-pVTZ.(unit:a.u.)

Molecules	0.7	0.8	0.9	1.0	1.25	1.5	2.0
CH_4-F_2	-56.505747/ 0.000108	-56.511537/ 0.000113	-56.512528/ 0.000114	-56.512799/ 0.000107	-56.512524/ 0.000111	-56.512348/ 0.000108	-56.512163/ 0.000111
CH_4-Cl2	-37.937325/ 0.000133	-37.955547/ 0.000138	-37.959847/ 0.000151	-37.959765/ 0.000134	-37.959164/ 0.000125	-37.958803/ 0.000122	-37.958508/ 0.000122
CH_4-Br_2	-34.782286/ 0.000121	-34.804605/ 0.000092	-34.810161/ 0.000104	-34.810602/ 0.000098	-34.80958/ 0.000091	-34.809261/ 0.000095	-34.808813/ 0.000094
CH_4-I_2	-30.956228/ 0.000105	-30.980719/ 0.000149	-30.986794/ 0.000092	-30.987536/ 0.000101	-30.986213/ 0.000091	-30.985855/ 0.00009	-30.985421/ 0.000124
CH_3F-CH_3F	-63.536298/ 0.000131	-63.552032/ 0.000116	-63.555375/ 0.000117	-63.555413/ 0.000129	-63.554408/ 0.000123	-63.553851/ 0.00012	-63.553472/ 0.000124
CH_3Cl-CH_3Cl	-44.851637/ 0.000148	-44.867811/ 0.000149	-44.871987/ 0.000165	-44.872509/ 0.000147	-44.871219/ 0.000145	-44.870513/ 0.000157	-44.870721/ 0.000136
CH_3F-CH_4	-39.847794/ 0.000104	-39.859398/ 0.000106	-39.861654/ 0.000108	-39.861561/ 0.000108	-39.861054/ 0.000097	-39.860613/ 0.000092	-39.860668/ 0.000094
CH_3Cl-CH_4	-30.496555/ 0.000129	-30.51625/ 0.000117	-30.520639/ 0.000117	-30.520764/ 0.00012	-30.519914/ 0.000115	-30.519427/ 0.000112	-30.519206/ 0.000113
CHF_3-CH_4	-87.288564/ 0.000138	-87.297475/ 0.00013	-87.298558/ 0.00013	-87.298743/ 0.00014	-87.298271/ 0.000129	-87.298064/ 0.000131	-87.298155/ 0.000132
$CHCl_3$-CH_4	-59.195642/ 0.000182	-59.214178/ 0.000178	-59.21848/ 0.000177	-59.219301/ 0.000174	-59.217845/ 0.00016	-59.217585/ 0.000175	-59.217397/ 0.000177