Supporting Material: Tables

**Table S1.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 0.942 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.112026 

3.4  0  0.066591

3.5  0  0.057969

3.6  0  0.050310

3.7  0  0.043532

3.8  0  0.037553

3.9  0  0.032292

4.0 0 0 0.027675 0.027675

4.2  0  0.020099

4.5  0  0.012009

5.0 0 0 0.004344 0.004344

6.0 0 0 0.000587 0.000587

7.0 0 0 0.001077 0.001077

8.0 0 0 0.000794 0.000789

9.0 0 0 0.000520 0.000520

10.0 0 0 0.000342 0.000342

R (a.u.), = 5° Y† Y Z†Z

3.0 0.001635  0.112300 

3.4  0.001180  0.066790

3.5  0.001093  0.058153

3.6  0.001014  0.050481

3.7  0.000943  0.043690

3.8  0.000877  0.037698

3.9  0.000817  0.032427

4.0 0.000761 0.000761 0.027799 0.027800

4.2  0.000663  0.020206

4.5  0.000540  0.012095

5.0 0.000388 0.000388 0.004403 0.004403

6.0 0.000206 0.000206 0.000558 0.000558

7.0 0.000114 0.000114 0.001061 0.001061

8.0 0.000067 0.000067 0.000785 0.000780

9.0 0.000042 0.000042 0.000515 0.000515

10.0 0.000027 0.000027 0.000338 0.000338

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.003212  0.113140 

3.4  0.002316  0.067382

3.5  0.002146  0.058700

3.6  0.001991  0.050986

3.7  0.001850  0.044157

3.8  0.001721  0.038131

3.9  0.001603  0.032827

4.0 0.001494 0.001494 0.028170 0.028170

4.2  0.001301  0.020524

4.5  0.001062  0.012347

5.0 0.000763 0.000763 0.004577 0.004577

6.0 0.000405 0.000405 0.000471 0.000471

7.0 0.000225 0.000225 0.001015 0.001015

8.0 0.000132 0.000133 0.000759 0.000768

9.0 0.000082 0.000083 0.000498 0.000498

10.0 0.000054 0.000054 0.000327 0.000327

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.004680  0.114491 

3.4  0.003374  0.068348

3.5  0.003125  0.059592

3.6  0.002899  0.051811

3.7  0.002694  0.044919

3.8  0.002506  0.038836

3.9  0.002334  0.033479

4.0 0.002177 0.002176 0.028774 0.028774

4.2  0.001896  0.021041

4.5  0.001548  0.012760

5.0 0.001113 0.001113 0.004860 0.004860

6.0 0.000592 0.000592 0.000331 0.000331

7.0 0.000328 0.000328 0.000939 0.000939

8.0 0.000194 0.000194 0.000715 0.000724

9.0 0.000121 0.000121 0.000471 0.000471

10.0 0.000079 0.000079 0.000309 0.000309

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.005991  0.116325 

3.4  0.004319  0.069655

3.5  0.004000  0.060799

3.6  0.003711  0.052926

3.7  0.003448  0.045951

3.8  0.003208  0.039790

3.9  0.002988  0.034362

4.0 0.002786 0.002786 0.029591 0.029591

4.2  0.002428  0.021741

4.5  0.001983  0.013310

5.0 0.001427 0.001427 0.005243 0.005242

6.0 0.000760 0.000760 0.000141 0.000141

7.0 0.000422 0.000422 0.000837 0.000837

8.0 0.000249 0.000249 0.000655 0.000664

9.0 0.000155 0.000155 0.000434 0.000433

10.0 0.000101 0.000101 0.000285 0.000285

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.007105  0.118590 

3.4  0.005123  0.071260

3.5  0.004745  0.062280

3.6  0.004403  0.054294

3.7  0.004091  0.047216

3.8  0.003806  0.040960

3.9  0.003546  0.035444

4.0 0.003306 0.003306 0.030592 0.030592

4.2  0.002882  0.022598

4.5  0.002355  0.014000

5.0 0.001696 0.001696 0.005711 0.005711

6.0 0.000903 0.000903 0.000092 0.000092

7.0 0.000502 0.000502 0.000711 0.000711

8.0 0.000297 0.000296 0.000583 0.000591

9.0 0.000184 0.000184 0.000389 0.000388

10.0 0.000120 0.000120 0.000256 0.000255

R (a.u.), = 30° Y† Y Z†Z

3.0 0.007986  0.121206 

3.4  0.005762  0.073111

3.5  0.005337  0.063987

3.6  0.004952  0.055871

3.7  0.004602  0.048673

3.8  0.004282  0.042306

3.9  0.003990  0.036689

4.0 0.003720 0.003720 0.031743 0.031743

4.2  0.003243  0.023584

4.5  0.002654  0.014783

5.0 0.001911 0.001911 0.006250 0.006250

6.0 0.001019 0.001019 0.000361 0.000361

7.0 0.000567 0.000567 0.000566 0.000566

8.0 0.000335 0.000335 0.000498 0.000507

9.0 0.000208 0.000208 0.000337 0.000336

10.0 0.000136 0.000136 0.000221 0.000221

R (a.u.), = 35° Y† Y Z†Z

3.0 0.008610  0.124103 

3.4  0.006216  0.075146

3.5  0.005759  0.065864

3.6  0.005344  0.057602

3.7  0.004967  0.050272

3.8  0.004623  0.043784

3.9  0.004307  0.038055

4.0 0.004017 0.004017 0.033007 0.033007

4.2  0.003503  0.024666

4.5  0.002865  0.015642

5.0 0.002066 0.002066 0.006841 0.006841

6.0 0.001103 0.001103 0.000656 0.000656

7.0 0.000614 0.000614 0.000406 0.000406

8.0 0.000363 0.000363 0.000406 0.000414

9.0 0.000225 0.000225 0.000279 0.000279

10.0 0.000147 0.000147 0.000184 0.000184

R (a.u.), = 40° Y† Y Z†Z

3.0 0.008962  0.127183 

3.4  0.006475  0.077303

3.5  0.006000  0.067849

3.6  0.005569  0.059433

3.7  0.005177  0.051962

3.8  0.004819  0.045345

3.9  0.004490  0.039498

4.0 0.004188 0.004188 0.034341 0.034341

4.2  0.003653  0.025808

4.5  0.002988  0.016539

5.0 0.002157 0.002156 0.007466 0.007466

6.0 0.001152 0.001152 0.000969 0.000969

7.0 0.000643 0.000643 0.000237 0.000237

8.0 0.000380 0.000380 0.000307 0.000316

9.0 0.000236 0.000236 0.000218 0.000217

10.0 0.000154 0.000154 0.000144 0.000143

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.009037  0.130351 

3.4  0.006534  0.079510

3.5  0.006056  0.069881

3.6  0.005622  0.061306

3.7  0.005227  0.053689

3.8  0.004866  0.046940

3.9  0.004535  0.040972

4.0 0.004230 0.004230 0.035704 0.035703

4.2  0.003690  0.026975

4.5  0.003020  0.017471

5.0 0.002181 0.002181 0.008104 0.008104

6.0 0.001166 0.001166 0.001290 0.001289

7.0 0.000651 0.000651 0.000063 0.000063

8.0 0.000386 0.000386 0.000206 0.000217

9.0 0.000239 0.000239 0.000155 0.000154

10.0 0.000156 0.000156 0.000102 0.000102

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.008838  0.133514 

3.4  0.006395  0.081702

3.5  0.005928  0.071896

3.6  0.005505  0.063161

3.7  0.005119  0.055401

3.8  0.004766  0.048520

3.9  0.004442  0.042431

4.0 0.004144 0.004144 0.037052 0.037052

4.2  0.003616  0.028132

4.5  0.002960  0.018388

5.0 0.002139 0.002139 0.008736 0.008736

6.0 0.001145 0.001145 0.001608 0.001608

7.0 0.000640 0.000640 0.000110 0.000110

8.0 0.000379 0.000379 0.000106 0.000116

9.0 0.000235 0.000235 0.000092 0.000091

10.0 0.000153 0.000153 0.000061 0.000061

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.008376  0.136580 

3.4  0.006066  0.083810

3.5  0.005624  0.073834

3.6  0.005223  0.064945

3.7  0.004858  0.057045

3.8  0.004523  0.050037

3.9  0.004217  0.043832

4.0 0.003935 0.003935 0.038346 0.038341

4.2  0.003436  0.029240

4.5  0.002812  0.019268

5.0 0.002032 0.002032 0.009344 0.009343

6.0 0.001090 0.001090 0.001914 0.001914

7.0 0.000610 0.000610 0.000278 0.000278

8.0 0.000361 0.000361 0.000008 0.000018

9.0 0.000224 0.000224 0.000031 0.000031

10.0 0.000146 0.000146 0.000021 0.000021

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.007671  0.139444 

3.4  0.005559  0.085775

3.5  0.005156  0.075637

3.6  0.004789  0.066606

3.7  0.004454  0.058576

3.8  0.004148  0.051451

3.9  0.003868  0.045138

4.0 0.003609 0.003614 0.039549 0.039554

4.2  0.003150  0.030257

4.5  0.002580  0.020085

5.0 0.001866 0.001866 0.009909 0.009908

6.0 0.001001 0.001001 0.002200 0.002200

7.0 0.000561 0.000561 0.000434 0.000434

8.0 0.000332 0.000333 0.000083 0.000073

9.0 0.000206 0.000206 0.000026 0.000026

10.0 0.000135 0.000135 0.000017 0.000017

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.006747  0.142020 

3.4  0.004893  0.087539

3.5  0.004538  0.077254

3.6  0.004216  0.068089

3.7  0.003922  0.059946

3.8  0.003653  0.052714

3.9  0.003406  0.046305

4.0 0.003179 0.003179 0.040626 0.040631

4.2  0.002775  0.031185

4.5  0.002274  0.020818

5.0 0.001645 0.001645 0.010415 0.010414

6.0 0.000884 0.000884 0.002456 0.002456

7.0 0.000495 0.000495 0.000575 0.000575

8.0 0.000294 0.000294 0.000166 0.000156

9.0 0.000182 0.000182 0.000078 0.000078

10.0 0.000119 0.000119 0.000051 0.000051

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.005633  0.144237 

3.4  0.004088  0.089050

3.5  0.003792  0.078642

3.6  0.003523  0.069366

3.7  0.003278  0.061117

3.8  0.003054  0.053792

3.9  0.002848  0.047300

4.0 0.002658 0.002658 0.041549 0.041548

4.2  0.002321  0.031974

4.5  0.001902  0.021445

5.0 0.001376 0.001376 0.010849 0.010848

6.0 0.000740 0.000740 0.002676 0.002676

7.0 0.000415 0.000415 0.000696 0.000696

8.0 0.000246 0.000246 0.000237 0.000229

9.0 0.000153 0.000153 0.000122 0.000122

10.0 0.000100 0.000100 0.000080 0.000081

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.004364  0.146038 

3.4  0.003169  0.090271

3.5  0.002940  0.079761

3.6  0.002732  0.070395

3.7  0.002542  0.062063

3.8  0.002368  0.054664

3.9  0.002208  0.048103

4.0 0.002061 0.002061 0.042292 0.042292

4.2  0.001800  0.032609

4.5  0.001475  0.021951

5.0 0.001068 0.001068 0.011199 0.011198

6.0 0.000575 0.000575 0.002853 0.002853

7.0 0.000322 0.000322 0.000794 0.000794

8.0 0.000191 0.000191 0.000294 0.000286

9.0 0.000119 0.000119 0.000158 0.000158

10.0 0.000078 0.000078 0.000104 0.000104

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.002977  0.147357 

3.4  0.002162  0.091167

3.5  0.002006  0.080582

3.6  0.001864  0.071148

3.7  0.001735  0.062756

3.8  0.001616  0.055303

3.9  0.001507  0.048692

4.0 0.001407 0.001407 0.042837 0.042836

4.2  0.001229  0.033075

4.5  0.001007  0.022321

5.0 0.000729 0.000729 0.011455 0.011455

6.0 0.000392 0.000392 0.002983 0.002983

7.0 0.000220 0.000220 0.000866 0.000866

8.0 0.000131 0.000131 0.000336 0.000329

9.0 0.000081 0.000081 0.000184 0.000185

10.0 0.000053 0.000053 0.000122 0.000122

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.001509  0.148168 

3.4  0.001096  0.091714

3.5  0.001017  0.081083

3.6  0.000945  0.071608

3.7  0.000879  0.063180

3.8  0.000819  0.055693

3.9  0.000764  0.049052

4.0 0.000713 0.000713 0.043169 0.043169

4.2  0.000623  0.033360

4.5  0.000511  0.022547

5.0 0.000370 0.000370 0.011612 0.011612

6.0 0.000199 0.000199 0.003062 0.003062

7.0 0.000112 0.000112 0.000910 0.000910

8.0 0.000066 0.000066 0.000362 0.000357

9.0 0.000041 0.000041 0.000200 0.000201

10.0 0.000027 0.000027 0.000133 0.000133

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.148440 

3.4  0  0.091898

3.5  0  0.081251

3.6  0  0.071763

3.7  0  0.063322

3.8  0  0.055824

3.9  0  0.049173

4.0 0 0 0.043281 0.043280

4.2  0  0.033455

4.5  0  0.022623

5.0 0 0 0.011664 0.011664

6.0 0 0 0.003089 0.003089

7.0 0 0 0.000925 0.000925

8.0 0 0 0.000371 0.000365

9.0 0 0 0.000206 0.000206

10.0 0 0 0.000136 0.000136

**Table S2.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 1.111 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.101942 

3.4  0  0.060432

3.5  0  0.052309

3.6  0  0.045067

3.7  0  0.038652

3.8  0  0.032999

3.9  0  0.028039

4.0 0 0 0.023702 0.023703

4.2  0  0.016643

4.5  0  0.009230

5.0 0 0 0.002443 0.002443

6.0 0 0 0.001493 0.001493

7.0 0 0 0.001552 0.001552

8.0 0 0 0.001067 0.001063

9.0 0 0 0.000688 0.000701

10.0 0 0 0.000451 0.000451

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.002158  0.102352 

3.4  0.001557  0.060724

3.5  0.001441  0.052579

3.6  0.001336  0.045317

3.7  0.001241  0.038884

3.8  0.001154  0.033213

3.9  0.001074  0.028237

4.0 0.001001 0.001001 0.023886 0.023886

4.2  0.000872  0.016800

4.5  0.000713  0.009354

5.0 0.000514 0.000514 0.002527 0.002527

6.0 0.000277 0.000277 0.001452 0.001452

7.0 0.000155 0.000155 0.001530 0.001530

8.0 0.000091 0.000091 0.001055 0.001050

9.0 0.000057 0.000057 0.000681 0.000693

10.0 0.000037 0.000037 0.000446 0.000446

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.004235  0.103552 

3.4  0.003056  0.061590

3.5  0.002828  0.053380

3.6  0.002622  0.046059

3.7  0.002434  0.039571

3.8  0.002264  0.033849

3.9  0.002108  0.028825

4.0 0.001965 0.001965 0.024430 0.024430

4.2  0.001713  0.017266

4.5  0.001401  0.009722

5.0 0.001012 0.001012 0.002777 0.002777

6.0 0.000544 0.000544 0.001331 0.001331

7.0 0.000304 0.000304 0.001466 0.001467

8.0 0.000180 0.000180 0.001018 0.001014

9.0 0.000112 0.000112 0.000658 0.000671

10.0 0.000073 0.000073 0.000431 0.000431

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.006160  0.105527 

3.4  0.004445  0.063002

3.5  0.004114  0.054686

3.6  0.003814  0.047267

3.7  0.003542  0.040689

3.8  0.003294  0.034884

3.9  0.003067  0.029783

4.0 0.002860 0.002860 0.025316 0.025316

4.2  0.002493  0.018023

4.5  0.002040  0.010321

5.0 0.001475 0.001475 0.003184 0.003184

6.0 0.000793 0.000793 0.001135 0.001135

7.0 0.000444 0.000444 0.001363 0.001363

8.0 0.000262 0.000262 0.000959 0.000954

9.0 0.000164 0.000164 0.000622 0.000634

10.0 0.000107 0.000107 0.000408 0.000407

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.007866  0.108213 

3.4  0.005679  0.064913

3.5  0.005257  0.056452

3.6  0.004875  0.048901

3.7  0.004527  0.042200

3.8  0.004211  0.036282

3.9  0.003922  0.031076

4.0 0.003658 0.003658 0.026512 0.026512

4.2  0.003190  0.019045

4.5  0.002612  0.011128

5.0 0.001890 0.001890 0.003733 0.003732

6.0 0.001016 0.001016 0.000869 0.000869

7.0 0.000569 0.000569 0.001222 0.001222

8.0 0.000336 0.000336 0.000878 0.000874

9.0 0.000210 0.000210 0.000572 0.000582

10.0 0.000137 0.000137 0.000375 0.000375

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.009298  0.111538 

3.4  0.006720  0.067261

3.5  0.006222  0.058620

3.6  0.005771  0.050903

3.7  0.005361  0.044051

3.8  0.004987  0.037993

3.9  0.004646  0.032658

4.0 0.004334 0.004334 0.027974 0.027974

4.2  0.003781  0.020294

4.5  0.003098  0.012115

5.0 0.002244 0.002244 0.004402 0.004404

6.0 0.001207 0.001207 0.000544 0.000544

7.0 0.000676 0.000676 0.001050 0.001050

8.0 0.000399 0.000399 0.000779 0.000775

9.0 0.000249 0.000249 0.000511 0.000521

10.0 0.000163 0.000163 0.000335 0.000335

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.010413  0.115388 

3.4  0.007535  0.069966

3.5  0.006979  0.061114

3.6  0.006475  0.053206

3.7  0.006017  0.046178

3.8  0.005600  0.039958

3.9  0.005218  0.034473

4.0 0.004868 0.004868 0.029651 0.029651

4.2  0.004249  0.021726

4.5  0. 003484  0.013245

5.0 0.002525 0.002525 0.005170 0.005175

6.0 0.001360 0.001360 0.000171 0.000171

7.0 0.000762 0.000762 0.000851 0.000851

8.0 0.000450 0.000450 0.000665 0.000660

9.0 0.000281 0.000281 0.000441 0.000451

10.0 0.000184 0.000184 0.000289 0.000289

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.011182  0.119656 

3.4  0.008104  0.072942

3.5  0.007509  0.063853

3.6  0.006969  0.055731

3.7  0.006479  0.048507

3.8  0.006031  0.042108

3.9  0.005621  0.036459

4.0 0.005246 0.005246 0.031486 0.031485

4.2  0.004581  0.023291

4.5  0.003758  0.014481

5.0 0.002727 0.002727 0.006010 0.006014

6.0 0.001470 0.001470 0.000239 0.000239

7.0 0.000824 0.000824 0.000633 0.000633

8.0 0.000487 0.000487 0.000539 0.000535

9.0 0.000304 0.000304 0.000363 0.000373

10.0 0.000199 0.000199 0.000239 0.000238

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.011590  0.124220 

3.4  0.008414  0.076090

3.5  0.007800  0.066747

3.6  0.007242  0.058396

3.7  0.006735  0.050964

3.8  0.006272  0.044374

3.9  0.005848  0.038550

4.0 0.005458 0.005458 0.033415 0.033415

4.2  0.004769  0.024937

4.5  0.003915  0.015779

5.0 0.002843 0.002843 0.006893 0.006894

6.0 0.001534 0.001534 0.000671 0.000671

7.0 0.000861 0.000861 0.000402 0.000402

8.0 0.000509 0.000509 0.000406 0.000401

9.0 0.000317 0.000317 0.000280 0.000290

10.0 0.000207 0.000207 0.000185 0.000184

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.011637  0.128919 

3.4  0.008463  0.079310

3.5  0.007848  0.069703

3.6  0.007290  0.061114

3.7  0.006782  0.053467

3.8  0.006318  0.046681

3.9  0.005893  0.040677

4.0 0.005502 0.005502 0.035379 0.035378

4.2  0.004810  0.026610

4.5  0.003951  0.017100

5.0 0.002871 0.002871 0.007791 0.007791

6.0 0.001551 0.001551 0.001113 0.001113

7.0 0.000871 0.000871 0.000166 0.000166

8.0 0.000516 0.000516 0.000269 0.000282

9.0 0.000321 0.000321 0.000195 0.000205

10.0 0.000210 0.000210 0.000129 0.000129

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.011333  0.133624 

3.4  0.008256  0.082502

3.5  0.007660  0.072629

3.6  0.007119  0.063802

3.7  0.006625  0.055940

3.8  0.006174  0.048958

3.9  0.005760  0.042776

4.0 0.005380 0.005380 0.037314 0.037314

4.2  0.004705  0.028259

4.5  0.003867  0.018401

5.0 0.002812 0.002812 0.008677 0.008677

6.0 0.001521 0.001521 0.001549 0.001549

7.0 0.000855 0.000855 0.000069 0.000069

8.0 0.000507 0.000507 0.000133 0.000146

9.0 0.000315 0.000315 0.000110 0.000120

10.0 0.000206 0.000206 0.000074 0.000073

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.010698  0.138190 

3.4  0.007807  0.085570

3.5  0.007247  0.075437

3.6  0.006737  0.066378

3.7  0.006272  0.058307

3.8  0.005847  0.051137

3.9  0.005457  0.044783

4.0 0.005098 0.005098 0.039164 0.039164

4.2  0.004461  0.029834

4.5  0.003668  0.019643

5.0 0.002670 0.002669 0.009525 0.009524

6.0 0.001446 0.001446 0.001968 0.001968

7.0 0.000813 0.000813 0.000295 0.000295

8.0 0.000482 0.000482 0.000002 0.000015

9.0 0.000300 0.000300 0.000028 0.000022

10.0 0.000196 0.000196 0.000020 0.000019

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.009761  0.142451 

3.4  0.007135  0.088422

3.5  0.006625  0.078045

3.6  0.006162  0.068769

3.7  0.005739  0.060502

3.8  0.005352  0.053156

3.9  0.004996  0.046642

4.0 0.004668 0.004669 0.040877 0.040877

4.2  0.004086  0.031292

4.5  0.003362  0.020793

5.0 0.002448 0.002448 0.010310 0.010309

6.0 0.001328 0.001328 0.002358 0.002357

7.0 0.000748 0.000748 0.000506 0.000506

8.0 0.000444 0.000444 0.000121 0.000108

9.0 0.000276 0.000276 0.000048 0.000055

10.0 0.000181 0.000181 0.000030 0.000031

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.008556  0.146308 

3.4  0.006264  0.090978

3.5  0.005819  0.080380

3.6  0.005414  0.070906

3.7  0.005043  0.062464

3.8  0.004704  0.054959

3.9  0.004393  0.048301

4.0 0.004106 0.004106 0.042406 0.042406

4.2  0.003595  0.032592

4.5  0.002959  0.021819

5.0 0.002156 0.002156 0.011011 0.011010

6.0 0.001170 0.001170 0.002706 0.002706

7.0 0.000660 0.000660 0.000696 0.000696

8.0 0.000392 0.000392 0.000231 0.000219

9.0 0.000244 0.000244 0.000117 0.000124

10.0 0.000159 0.000159 0.000076 0.000076

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.007124  0.149619 

3.4  0.005222  0.093168

3.5  0.004853  0.082377

3.6  0.004516  0.072734

3.7  0.004208  0.064140

3.8  0.003926  0.056499

3.9  0.003667  0.049718

4.0 0.003428 0.003428 0.043711 0.043710

4.2  0.003003  0.033702

4.5  0.002473  0.022701

5.0 0.001803 0.001803 0.011609 0.011609

6.0 0.000979 0.000979 0.003004 0.003004

7.0 0.000552 0.000552 0.000858 0.000858

8.0 0.000328 0.000328 0.000326 0.000314

9.0 0.000204 0.000204 0.000176 0.000183

10.0 0.000134 0.000134 0.000115 0.000116

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.005507  0.152308 

3.4  0.004041  0.094932

3.5  0.003756  0.083985

3.6  0.003496  0.074205

3.7  0.003259  0.065488

3.8  0.003041  0.057737

3.9  0.002841  0.050856

4.0 0.002656 0.002656 0.044759 0.044759

4.2  0.002327  0.034594

4.5  0.001919  0.023404

5.0 0.001398 0.001398 0.012090 0.012090

6.0 0.000760 0.000760 0.003244 0.003243

7.0 0.000429 0.000429 0.000990 0.000989

8.0 0.000255 0.000255 0.000403 0.000390

9.0 0.000159 0.000159 0.000224 0.000231

10.0 0.000104 0.000104 0.000147 0.000148

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.003749  0.154284 

3.4  0.002754  0.096225

3.5  0.002560  0.085163

3.6  0.002383  0.075281

3.7  0.002222  0.066475

3.8  0.002074  0.058642

3.9  0.001937  0.051689

4.0 0.001811 0.001811 0.045526 0.045526

4.2  0.001587  0.035246

4.5  0.001308  0.023905

5.0 0.000954 0.000954 0.012442 0.012442

6.0 0.000519 0.000519 0.003419 0.003419

7.0 0.000293 0.000293 0.001086 0.001086

8.0 0.000174 0.000174 0.000459 0.000447

9.0 0.000108 0.000109 0.000260 0.000266

10.0 0.000071 0.000071 0.000170 0.000171

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.001898  0.155492 

3.4  0.001395  0.097014

3.5  0.001297  0.085882

3.6  0.001207  0.075938

3.7  0.001126  0.067076

3.8  0.001051  0.059195

3.9  0.000982  0.052197

4.0 0.000918 0.000918 0.045993 0.045993

4.2  0.000805  0.035643

4.5  0.000663  0.024228

5.0 0.000484 0.000484 0.012657 0.012657

6.0 0.000263 0.000263 0.003526 0.003526

7.0 0.000149 0.000149 0.001145 0.001145

8.0 0.000088 0.000088 0.000494 0.000481

9.0 0.000055 0.000055 0.000281 0.000288

10.0 0.000036 0.000036 0.000185 0.000185

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.155900 

3.4  0  0.097279

3.5  0  0.086123

3.6  0  0.076159

3.7  0  0.067278

3.8  0  0.059380

3.9  0  0.052367

4.0 0 0 0.046150 0.046150

4.2  0  0.035776

4.5  0  0.024333

5.0 0 0 0.012729 0.012729

6.0 0 0 0.003562 0.003562

7.0 0 0 0.001164 0.001164

8.0 0 0 0.000506 0.000493

9.0 0 0 0.000289 0.000295

10.0 0 0 0.000190 0.000190

**Table S3.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 1.280 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.087531 

3.4  0  0.052001

3.5  0  0.044625

3.6  0  0.038001

3.7  0  0.032114

3.8  0  0.026929

3.9  0  0.022395

4.0 0 0 0.018453 0.018453

4.2  0  0.012111

4.5  0  0.005628

5.0 0 0 0.000036 0.000036

6.0 0 0 0.002573 0.002573

7.0 0 0 0.002089 0.002089

8.0 0 0 0.001367 0.001368

9.0 0 0 0.000871 0.000873

10.0 0 0 0.000569 0.000569

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.002698  0.088081 

3.4  0.001959  0.052401

3.5  0.001812  0.044998

3.6  0.001678  0.038347

3.7  0.001556  0.032436

3.8  0.001445  0.027228

3.9  0.001345  0.022672

4.0 0.001253 0.001253 0.018710 0.018710

4.2  0.001092  0.012331

4.5  0.000895  0.005802

5.0 0.000649 0.000649 0.000153 0.000153

6.0 0.000353 0.000353 0.002518 0.002518

7.0 0.000200 0.000199 0.002061 0.002061

8.0 0.000118 0.000118 0.001352 0.001352

9.0 0.000074 0.000074 0.000861 0.000863

10.0 0.000048 0.000048 0.000563 0.000563

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.005289  0.089711 

3.4  0.003841  0.053590

3.5  0.003551  0.046102

3.6  0.003288  0.039374

3.7  0.003050  0.033390

3.8  0.002834  0.028114

3.9  0.002637  0.023493

4.0 0.002458 0.002458 0.019471 0.019471

4.2  0.002143  0.012982

4.5  0.001756  0.006315

5.0 0.001275 0.001275 0.000498 0.000498

6.0 0.000693 0.000693 0.002356 0.002356

7.0 0.000392 0.000392 0.001977 0.001977

8.0 0.000232 0.000232 0.001304 0.001305

9.0 0.000145 0.000145 0.000832 0.000835

10.0 0.000095 0.000095 0.000544 0.000544

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.007673  0.092378 

3.4  0.005575  0.055530

3.5  0.005156  0.047905

3.6  0.004776  0.041048

3.7  0.004431  0.034944

3.8  0.004118  0.029555

3.9  0.003833  0.024830

4.0 0.003573 0.003573 0.020708 0.020708

4.2  0.003116  0.014041

4.5  0.002555  0.007149

5.0 0.001857 0.001857 0.001059 0.001059

6.0 0.001009 0.001009 0.002092 0.002093

7.0 0.000570 0.000570 0.001841 0.001841

8.0 0.000337 0.000337 0.001227 0.001228

9.0 0.000211 0.000211 0.000785 0.000788

10.0 0.000138 0.000138 0.000514 0.000514

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.009764  0.096032 

3.4  0.007103  0.058161

3.5  0.006572  0.050344

3.6  0.006090  0.043310

3.7  0.005652  0.037042

3.8  0.005255  0.031500

3.9  0.004893  0.026630

4.0 0.004562 0.004562 0.022375 0.022375

4.2  0.003980  0.015465

4.5  0.003266  0.008271

5.0 0.002376 0.002376 0.001812 0.001812

6.0 0.001292 0.001292 0.001737 0.001737

7.0 0.000729 0.000729 0.001657 0.001657

8.0 0.000432 0.000432 0.001123 0.001123

9.0 0.000270 0.000270 0.000722 0.000718

10.0 0.000177 0.000177 0.000472 0.000469

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.011489  0.100577 

3.4  0.008374  0.061393

3.5  0.007753  0.053337

3.6  0.007188  0.046082

3.7  0.006675  0.039609

3.8  0.006209  0.033877

3.9  0.005783  0.028830

4.0 0.005394 0.005394 0.024409 0.024409

4.2  0.004709  0.017202

4.5  0.003868  0.009638

5.0 0.002817 0.002817 0.002730 0.002730

6.0 0.001532 0.001532 0.001303 0.001303

7.0 0.000865 0.000865 0.001432 0.001432

8.0 0.000512 0.000512 0.000994 0.000994

9.0 0.000320 0.000320 0.000643 0.000640

10.0 0.000209 0.000210 0.000421 0.000418

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.012798  0.105896 

3.4  0.009351  0.065131

3.5  0.008664  0.056787

3.6  0.008038  0.049270

3.7  0.007469  0.042556

3.8  0.006951  0.036601

3.9  0.006478  0.031348

4.0 0.006045 0.006045 0.026735 0.026736

4.2  0.005282  0.019187

4.5  0.004342  0.011198

5.0 0.003166 0.003166 0.003778 0.003778

6.0 0.001724 0.001724 0.000806 0.000806

7.0 0.000973 0.000973 0.001172 0.001172

8.0 0.000576 0.000576 0.000846 0.000846

9.0 0.000360 0.000360 0.000552 0.000549

10.0 0.000236 0.000236 0.000362 0.000359

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.013662  0.111826 

3.4  0.010012  0.069249

3.5  0.009283  0.060576

3.6  0.008619  0.052764

3.7  0.008015  0.045780

3.8  0.007464  0.039577

3.9  0.006960  0.034096

4.0 0.006498 0.006498 0.029272 0.029273

4.2  0.005683  0.021347

4.5  0.004677  0.012896

5.0 0.003415 0.003415 0.004919 0.004919

6.0 0.001861 0.001861 0.000263 0.000263

7.0 0.001050 0.001050 0.000888 0.000888

8.0 0.000622 0.000622 0.000684 0.000684

9.0 0.000388 0.000389 0.000452 0.000449

10.0 0.000255 0.000255 0.000298 0.000294

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.014073  0.118211 

3.4  0.010345  0.073607

3.5  0.009600  0.064578

3.6  0.008921  0.056446

3.7  0.008302  0.049173

3.8  0.007737  0.042705

3.9  0.007219  0.036980

4.0 0.006744 0.006744 0.031932 0.031932

4.2  0.005903  0.023610

4.5  0.004864  0.014672

5.0 0.003555 0.003555 0.006113 0.006113

6.0 0.001941 0.001941 0.000307 0.000307

7.0 0.001096 0.001096 0.000588 0.000588

8.0 0.000649 0.000649 0.000512 0.000511

9.0 0.000405 0.000406 0.000346 0.000343

10.0 0.000266 0.000266 0.000229 0.000225

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.014040  0.124835 

3.4  0.010355  0.078068

3. 5  0.009618  0.068665

3.6  0.008945  0.060199

3.7  0.008331  0.052624

3.8  0.007769  0.045881

3.9  0.007254  0.039905

4.0 0.006780 0.006780 0.034627 0.034628

4.2  0.005941  0.025900

4.5  0.004900  0.016469

5.0 0.003586 0.003586 0.007322 0.007321

6.0 0.001960 0.001960 0.000887 0.000887

7.0 0.001107 0.001107 0.000281 0.000281

8.0 0.000657 0.000657 0.000335 0.000335

9.0 0.000410 0.000410 0.000237 0.000234

10.0 0.000269 0.000269 0.000158 0.000154

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.013586  0.131504 

3.4  0.010055  0.082492

3.5  0.009347  0.072708

3.6  0.008701  0.063903

3.7  0.008110  0.056023

3.8  0.007568  0.049006

3.9  0.007070  0.042780

4.0 0.006613 0.006613 0.037274 0.037274

4.2  0.005800  0.028146

4.5  0.004788  0.018230

5.0 0.003509 0.003508 0.008507 0.008507

6.0 0.001921 0.001921 0.001459 0.001458

7.0 0.001086 0.001086 0.000022 0.000022

8.0 0.000644 0.000644 0.000161 0.000160

9.0 0.000402 0.000402 0.000129 0.000125

10.0 0.000264 0.000264 0.000087 0.000083

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.012746  0.137984 

3.4  0.009465  0.086742

3.5  0.008807  0.076583

3.6  0.008204  0.067446

3.7  0.007653  0.059271

3.8  0.007146  0.051987

3.9  0.006680  0.045520

4.0 0.006251 0.006251 0.039794 0.039794

4.2  0.005487  0.030283

4.5  0.004535  0.019904

5.0 0.003327 0.003326 0.009636 0.009635

6.0 0.001824 0.001824 0.002005 0.002005

7.0 0.001032 0.001032 0.000313 0.000313

8.0 0.000613 0.000613 0.000007 0.000008

9.0 0.000382 0.000383 0.000024 0.000021

10.0 0.000251 0.000251 0.000018 0.000015

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.011564  0.144083 

3.4  0.008615  0.090691

3.5  0.008022  0.080176

3.6  0.007479  0.070727

3.7  0.006981  0.062273

3.8  0.006523  0.054740

3.9  0.006101  0.048047

4.0 0.005711 0.005712 0.042117 0.042117

4.2  0.005018  0.032250

4.5  0.004150  0.021445

5.0 0.003047 0.003041 0.010676 0.010681

6.0 0.001673 0.001673 0.002510 0.002510

7.0 0.000948 0.000948 0.000583 0.000583

8.0 0.000563 0.000563 0.000164 0.000164

9.0 0.000351 0.000352 0.000074 0.000077

10.0 0.000230 0.000230 0.000046 0.000049

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.010085  0.149598 

3.4  0.007536  0.094227

3.5  0.007022  0.083388

3.6  0.006551  0.073654

3.7  0.006118  0.064949

3.8  0.005720  0.057191

3.9  0.005353  0.050296

4.0 0.005013 0.005013 0.044183 0.044183

4.2  0.004407  0.033998

4.5  0.003648  0.022815

5.0 0.002681 0.002681 0.011600 0.011599

6.0 0.001473 0.001473 0.002960 0.002960

7.0 0.000836 0.000836 0.000825 0.000825

8.0 0.000497 0.000497 0.000304 0.000304

9.0 0.000310 0.000310 0.000161 0.000165

10.0 0.000203 0.000203 0.000104 0.000107

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.008360  0.154363 

3.4  0.006263  0.097253

3.5  0.005840  0.086132

3.6  0.005451  0.076152

3.7  0.005094  0.067230

3.8  0.004764  0.059278

3.9  0.004460  0.052209

4.0 0.004179 0.004179 0.045940 0.045940

4.2  0.003676  0.035485

4.5  0.003045  0.023978

5.0 0.002239 0.002239 0.012387 0.012386

6.0 0.001232 0.001232 0.003345 0.003345

7.0 0.000699 0.000699 0.001033 0.001033

8.0 0.000416 0.000416 0.000425 0.000425

9.0 0.000259 0.000260 0.000237 0.000240

10.0 0.000170 0.000170 0.000153 0.000156

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.006440  0.158223 

3.4  0.004834  0.099688

3.5  0.004510  0.088338

3.6  0.004212  0.078158

3.7  0.003937  0.069060

3.8  0.003684  0.060952

3.9  0.003450  0.053743

4.0 0.003233 0.003233 0.047348 0.047348

4.2  0.002845  0.036675

4.5  0.002358  0.024910

5.0 0.001735 0.001735 0.013017 0.013016

6.0 0.000955 0.000955 0.003654 0.003654

7.0 0.000543 0.000543 0.001200 0.001200

8.0 0.000323 0.000323 0.000522 0.000522

9.0 0.000202 0.000202 0.000297 0.000301

10.0 0.000132 0.000132 0.000194 0.000197

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.004373  0.161067 

3.4  0.003289  0.101471

3.5  0.003069  0.089951

3.6  0.002867  0.079624

3.7  0.002681  0.070397

3.8  0.002509  0.062174

3.9  0.002350  0.054863

4.0 0.002203 0.002203 0.048375 0.048375

4.2  0.001939  0.037543

4.5  0.001608  0.025582

5.0 0.001183 0.001183 0.013477 0.013476

6.0 0.000652 0.000652 0.003880 0.003880

7.0 0.000371 0.000371 0.001322 0.001322

8.0 0.000221 0.000221 0.000593 0.000593

9.0 0.000138 0.000138 0.000342 0.000346

10.0 0.000090 0.000090 0.000223 0.000226

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.002211  0.162802 

3.4  0.001664  0.102559

3.5  0.001553  0.090935

3.6  0.001451  0.080518

3.7  0.001357  0.071211

3.8  0.001270  0.062918

3.9  0.001190  0.055544

4.0 0.001116 0.001116 0.049000 0.049000

4.2  0.000982  0.038071

4.5  0.000818  0.026011

5.0 0.000600 0.000600 0.013757 0.013756

6.0 0.000331 0.000331 0.004017 0.004017

7.0 0.000188 0.000188 0.001397 0.001397

8.0 0.000112 0.000112 0.000637 0.000637

9.0 0.000070 0.000070 0.000369 0.000373

10.0 0.000046 0.000046 0.000241 0.000244

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.163388 

3.4  0  0.102924

3.5  0  0.091265

3.6  0  0.080818

3.7  0  0.071484

3.8  0  0.063167

3.9  0  0.055773

4.0 0 0 0.049210 0.049210

4.2  0  0.038248

4.5  0  0.026149

5.0 0 0 0.013851 0.013850

6.0 0 0 0.004064 0.004064

7.0 0 0 0.001422 0.001422

8.0 0 0 0.000652 0.000652

9.0 0 0 0.000379 0.000382

10.0 0 0 0.000248 0.000251

**Table S4.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 1.449 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.068855 

3.4  0  0.041384

3.5  0  0.034992

3.6  0  0.029165

3.7  0  0.023943

3.8  0  0.019363

3.9  0  0.015357

4.0 0 0 0.011906 0.011907

4.2  0  0.006465

4.5  0  0.001161

5.0 0 0 0.002905 0.002904

6.0 0 0 0.003829 0.003829

7.0 0 0 0.002683 0.002683

8.0 0 0 0.001689 0.001690

9.0 0 0 0.001064 0.001069

10.0 0 0 0.000693 0.000696

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.003223  0.069519 

3.4  0.002378  0.041898

3.5  0.002197  0.035475

3.6  0.002031  0.029618

3.7  0.001881  0.024368

3.8  0.001744  0.019759

3.9  0.001621  0.015725

4.0 0.001509 0.001508 0.012250 0.012251

4.2  0.001313  0.006761

4.5  0.001077  0.001395

5.0 0.000786 0.000786 0.002749 0.002749

6.0 0.000432 0.000432 0.003758 0.003758

7.0 0.000246 0.000246 0.002647 0.002647

8.0 0.000146 0.000146 0.001669 0.001670

9.0 0.000091 0.000091 0.001051 0.001057

10.0 0.000059 0.000060 0.000685 0.000688

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.006305  0.071520 

3.4  0.004655  0.043425

3.5  0.004302  0.036908

3.6  0.003978  0.030961

3.7  0.003685  0.025636

3.8  0.003412  0.020934

3.9  0.003177  0.016822

4.0 0.002957 0.002957 0.013269 0.013269

4.2  0.002575  0.007638

4.5  0.002112  0.002087

5.0 0.001542 0.001542 0.002288 0.002287

6.0 0.000848 0.000848 0.003547 0.003547

7.0 0.000482 0.000482 0.002541 0.002541

8.0 0.000286 0.000286 0.001610 0.001611

9.0 0.000178 0.000178 0.001016 0.001021

10.0 0.000117 0.000118 0.000662 0.000665

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.009114  0.074838 

3.4  0.006740  0.045925

3.5  0.006231  0.039249

3.6  0.005766  0.033153

3.7  0.005343  0.027682

3.8  0.004959  0.022845

3.9  0.004611  0.018593

4.0 0.004294 0.004294 0.014923 0.014923

4.2  0.003741  0.009059

4.5  0.003070  0.003208

5.0 0.002243 0.002243 0.001540 0.001539

6.0 0.001234 0.001234 0.003205 0.003205

7.0 0.000702 0.000702 0.002368 0.002369

8.0 0.000416 0.000416 0.001513 0.001515

9.0 0.000260 0.000260 0.000957 0.000963

10.0 0.000170 0.000171 0.000625 0.000614

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.011538  0.079425 

3.4  0.008552  0.049329

3.5  0.007914  0.042428

3.6  0.007329  0.036120

3.7  0.006797  0.030449

3.8  0.006313  0.025422

3.9  0.005873  0.020991

4.0 0.005472 0.005472 0.017149 0.017149

4.2  0.004772  0.010969

4.5  0.003921  0.004713

5.0 0.002868 0.002867 0.000537 0.000537

6.0 0.001578 0.001578 0.002744 0.002745

7.0 0.000897 0.000897 0.002135 0.002135

8.0 0.000532 0.000532 0.001383 0.001382

9.0 0.000332 0.000332 0.000878 0.000872

10.0 0.000217 0.000218 0.000573 0.000563

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.013487  0.085214 

3.4  0.010031  0.053541

3.5  0.009292  0.046347

3.6  0.008614  0.039767

3.7  0.007996  0.033842

3.8  0.007434  0.028575

3.9  0.006921  0.023918

4.0 0.006454 0.006454 0.019862 0.019862

4.2  0.005635  0.013292

4.5  0.004636  0.006541

5.0 0.003395 0.003395 0.000680 0.000681

6.0 0.001870 0.001870 0.002184 0.002184

7.0 0.001063 0.001063 0.001850 0.001851

8.0 0.000630 0.000630 0.001223 0.001223

9.0 0.000394 0.000394 0.000781 0.000775

10.0 0.000258 0.000259 0.000511 0.000500

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.014908  0.092080 

3.4  0.011134  0.058430

3.5  0.010327  0.050876

3.6  0.009586  0.043968

3.7  0.008908  0.037738

3.8  0.008290  0.032177

3.9  0.007726  0.027275

4.0 0.007211 0.007211 0.022959 0.022960

4.2  0.006305  0.015938

4.5  0.005195  0.008620

5.0 0.003811 0.003811 0.002064 0.002065

6.0 0.002101 0.002101 0.001544 0.001544

7.0 0.001194 0.001194 0.001524 0.001524

8.0 0.000708 0.000708 0.001038 0.001038

9.0 0.000442 0.000442 0.000669 0.000662

10.0 0.000290 0.000291 0.000438 0.000428

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.015777  0.099876 

3.4  0.011841  0.063843

3.5  0.010998  0.055870

3.6  0.010223  0.048583

3.7  0.009513  0.042005

3.8  0.008863  0.036122

3.9  0.008269  0.030921

4.0 0.007725 0.007724 0.026329 0.026329

4.2  0.006765  0.018810

4.5  0.005584  0.010871

5.0 0.004104 0.004104 0.003563 0.003564

6.0 0.002266 0.002266 0.000849 0.000849

7.0 0.001288 0.001288 0.001166 0.001167

8.0 0.000764 0.000764 0.000836 0.000836

9.0 0.000477 0.000478 0.000545 0.000538

10.0 0.000313 0.000314 0.000358 0.000348

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.016100  0.108343 

3.4  0.012150  0.069603

3.5  0.011302  0.061162

3.6  0.010521  0.053454

3.7  0.009804  0.046494

3.8  0.009146  0.040263

3.9  0.008542  0.034740

4.0 0.007988 0.007988 0.029852 0.029853

4.2  0.007008  0.021805

4.5  0.005795  0.013215

5.0 0.004267 0.004267 0.005123 0.005123

6.0 0.002360 0.002360 0.000121 0.000131

7.0 0.001342 0.001342 0.000791 0.000791

8.0 0.000797 0.000796 0.000622 0.000622

9.0 0.000498 0.000498 0.000414 0.000407

10.0 0.000326 0.000327 0.000273 0.000263

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.015905  0.117267 

3.4  0.012076  0.075525

3.5  0.011251  0.066577

3.6  0.010490  0.058421

3.7  0.009788  0.051059

3.8  0.009143  0.044463

3.9  0.008549  0.038605

4.0 0.008003 0.008003 0.033411 0.033412

4.2  0.007032  0.024824

4.5  0.005826  0.015573

5.0 0.004298 0.004298 0.006694 0.006694

6.0 0.002381 0.002381 0.000614 0.000614

7.0 0.001355 0.001355 0.000409 0.000409

8.0 0.000805 0.000805 0.000404 0.000404

9.0 0.000503 0.000503 0.000280 0.000273

10.0 0.000330 0.000331 0.000186 \*0.000176

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.015239  0.126328 

3.4  0.011644  0.081413

3.5  0.010867  0.071942

3.6  0.010147  0.063324

3.7  0.009481  0.055551

3.8  0.008867  0.048586

3.9  0.008301  0.042392

4.0 0.007778 0.007778 0.036893 0.036894

4.2  0.006846  0.027771

4.5  0.005682  0.017881

5.0 0.004199 0.004199 0.008225 0.008225

6.0 0.002330 0.002330 0.001336 0.001336

7.0 0.001327 0.001327 0.000032 0.000032

8.0 0.000789 0.000789 0.000189 0.000189

9.0 0.000493 0.000493 0.000147 0.000140

10.0 0.000323 0.000324 0.000099 0.000089

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.014161  0.135236 

3.4  0.010890  0.087081

3.5  0.010179  0.077086

3.6  0.009518  0.068012

3.7  0.008906  0.059835

3.8  0.008339  0.052515

3.9  0.007815  0.045984

4.0 0.007329 0.007329 0.040196 0.040197

4.2  0.006461  0.030560

4.5  0.005371  0.020036

5.0 0.003976 0.003976 0.009674 0.009674

6.0 0.002210 0.002210 0.002022 0.002022

7.0 0.001260 0.001260 0.000328 0.000338

8.0 0.000750 0.000750 0.000018 0.000018

9.0 0.000468 0.000468 0.000018 0.000012

10.0 0.000307 0.000308 0.000015 0.000007

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.012731  0.143668 

3.4  0.009852  0.092354

3.5  0.009222  0.081857

3.6  0.008635  0.072347

3.7  0.008089  0.063788

3.8  0.007583  0.056127

3.9  0.007113  0.049293

4.0 0.006677 0.006677 0.043229 0.043229

4.2  0.005894  0.033117

4.5  0.004907  0.022026

5.0 0.003638 0.003638 0.011002 0.011002

6.0 0.002025 0.002025 0.002654 0.002654

7.0 0.001156 0.001156 0.000662 0.000662

8.0 0.000689 0.000688 0.000210 0.000210

9.0 0.000430 0.000430 0.000101 0.000108

10.0 0.000282 0.000283 0.000063 0.000072

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.011012  0.151335 

3.4  0.008572  0.097076

3.5  0.008034  0.086118

3.6  0.007532  0.076210

3.7  0.007064  0.067303

3.8  0.006628  0.059333

3.9  0.006223  0.052228

4.0 0.005846 0.005846 0.045915 0.045915

4.2  0.005167  0.035378

4.5  0.004307  0.023789

5.0 0.003197 0.003197 0.012176 0.012176

6.0 0.001782 0.001782 0.003215 0.003215

7.0 0.001019 0.001019 0.000960 0.000960

8.0 0.000607 0.000607 0.000382 0.000382

9.0 0.000379 0.000379 0.000208 0.000215

10.0 0.000249 0.000250 0.000133 0.000142

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.009065  0.157986 

3.4  0.007092  0.101115

3.5  0.006655  0.089755

3.6  0.006245  0.079501

3.7  0.005863  0.070291

3.8  0.005506  0.062056

3.9  0.005173  0.054715

4.0 0.004862 0.004862 0.048191 0.048191

4.2  0.004302  0.037291

4.5  0.003590  0.025279

5.0 0.002667 0.002667 0.013171 0.013171

6.0 0.001488 0.001488 0.003693 0.003692

7.0 0.000852 0.000852 0.001214 0.001214

8.0 0.000508 0.000508 0.000529 0.000529

9.0 0.000318 0.000318 0.000300 0.000307

10.0 0.000209 0.000209 0.000194 0.000203

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.006942  0.163386 

3.4  0.005455  0.104365

3.5  0.005123  0.092675

3.6  0.004812  0.082139

3.7  0.004521  0.072685

3.8  0.004248  0.064234

3.9  0.003993  0.056702

4.0 0.003755 0.003754 0.050009 0.050007

4.2  0.003325  0.038819

4.5  0.002777  0.026466

5.0 0.002065 0.002065 0.013964 0.013964

6.0 0.001154 0.001153 0.004075 0.004075

7.0 0.000661 0.000661 0.001419 0.001419

8.0 0.000394 0.000394 0.000647 0.000647

9.0 0.000247 0.000247 0.000374 0.000381

10.0 0.000162 0.000163 0.000243 0.000252

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.004695  0.167361 

3.4  0.003701  0.106743

3.5  0.003478  0.094809

3.6  0.003268  0.084063

3.7  0.003073  0.074429

3.8  0.002889  0.065820

3.9  0.002717  0.058149

4.0 0.002556 0.002556 0.051332 0.051331

4.2  0.002264  0.039930

4.5  0.001892  0.027329

5.0 0.001408 0.001399 0.014542 0.014542

6.0 0.000787 0.000787 0.004354 0.004354

7.0 0.000451 0.000451 0.001568 0.001568

8.0 0.000269 0.000269 0.000734 0.000734

9.0 0.000168 0.000168 0.000428 0.000435

10.0 0.000111 0.000111 0.000279 0.000288

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.002367  0.169807 

3.4  0.001870  0.108191

3.5  0.001758  0.096107

3.6  0.001653  0.085235

3.7  0.001554  0.075490

3.8  0.001462  0.066784

3.9  0.001375  0.059028

4.0 0.001293 0.001294 0.052136 0.052135

4.2  0.001146  0.040604

4.5  0.000958  0.027853

5.0 0.000713 0.000713 0.014893 0.014893

6.0 0.000399 0.000399 0.004523 0.004523

7.0 0.000229 0.000229 0.001660 0.001659

8.0 0.000137 0.000136 0.000787 0.000787

9.0 0.000085 0.000085 0.000462 0.000469

10.0 0.000056 0.000057 0.000301 0.000310

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.170623 

3.4  0  0.108678

3.5  0  0.096544

3.6  0  0.085628

3.7  0  0.075846

3.8  0  0.067108

3.9  0  0.059323

4.0 0 0 0.052405 0.052404

4.2  0  0.040830

4.5  0  0.028028

5.0 0 0 0.015011 0.015010

6.0 0 0 0.004580 0.004580

7.0 0 0 0.001690 0.001690

8.0 0 0 0.000805 0.000805

9.0 0 0 0.000473 0.000480

10.0 0 0 0.000308 0.000317

**Table S5.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 1.618 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.046922 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0  0.004188 

4.2    

4.5    

5.0 0  0.006399 

6.0 0  0.005262 

7.0 0  0.003327 

8.0 0  0.002027 

9.0 0  0.001262 

10.0 0  0.000820 

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.003690  0.047645 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.001769  0.004628 

4.2    

4.5    

5.0 0.000918  0.006196 

6.0 0.000511  0.005171 

7.0 0.000293  0.003283 

8.0 0.000174  0.002002 

9.0 0.000108  0.001247 

10.0 0.000071  0.000811 

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.007196  0.049825 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.003465  0.005931 

4.2    

4.5    

5.0 0.001802  0.005595 

6.0 0.001003  0.004904 

7.0 0.000575  0.003151 

8.0 0.000341  0.001930 

9.0 0.000213  0.001204 

10.0 0.000139  0.000783 

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.010347  0.053496 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.005021  0.008046 

4.2    

4.5    

5.0 0.002621  0.004623 

6.0 0.001460  0.004470 

7.0 0.000836  0.002938 

8.0 0.000496  0.001812 

9.0 0.000309  0.001134 

10.0 0.000202  0.000738 

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.013000  0.058688 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.006379  0.010895 

4.2    

4.5    

5.0 0.003347  0.003323 

6.0 0.001866  0.003888 

7.0 0.001068  0.002651 

8.0 0.000634  0.001654 

9.0 0.000396  0.001039 

10.0 0.000259  0.000676 

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.015051  0.065409 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.007493  0.014367 

4.2    

4.5    

5.0 0.003959  0.001751 

6.0 0.002209  0.003183 

7.0 0.001265  0.002301 

8.0 0.000751  0.001459 

9.0 0.000469  0.000922 

10.0 0.000307  0.000601 

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.016445  0.073606 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.008333  0.018333 

4.2    

4.5    

5.0 0.004437  0.000028 

6.0 0.002480  0.002381 

7.0 0.001420  0.001900 

8.0 0.000844  0.001236 

9.0 0.000527  0.000787 

10.0 0.000345  0.000514 

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.017173  0.083154 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.008883  0.022646 

4.2    

4.5    

5.0 0.004771  0.001944 

6.0 0.002671  0.001513 

7.0 0.001530  0.001464 

8.0 0.000910  0.000992 

9.0 0.000568  0.000639 

10.0 0.000372  0.000419 

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.017266  0.093813 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.009139  0.027150 

4.2    

4.5    

5.0 0.004952  0.003927 

6.0 0.002778  0.000611 

7.0 0.001592  0.001007 

8.0 0.000948  0.000736 

9.0 0.000592  0.000482 

10.0 0.000388  0.000317 

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.016788  0.105284 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.009110  0.031692 

4.2    

4.5    

5.0 0.004980  0.005910 

6.0 0.002799  0.000297 

7.0 0.001606  0.000545 

8.0 0.000957  0.000474 

9.0 0.000598  0.000322 

10.0 0.000392  0.000214 

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.015823  0.117154 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.008812  0.036126 

4.2    

4.5    

5.0 0.004857  0.007832 

6.0 0.002736  0.001182 

7.0 0.001572  0.000091 

8.0 0.000937  0.000217 

9.0 0.000586  0.000163 

10.0 0.000384  0.000111 

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.014463  0.129004 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.008266  0.040317 

4.2    

4.5    

5.0 0.004592  0.009638 

6.0 0.002592  0.002020 

7.0 0.001491  0.000342 

8.0 0.000890  0.000030 

9.0 0.000557  0.000011 

10.0 0.000365  0.000011 

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.012798  0.140356 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.007501  0.044153 

4.2    

4.5    

5.0 0.004195  0.011283 

6.0 0.002372  0.002786 

7.0 0.001366  0.000741 

8.0 0.000816  0.000258 

9.0 0.000511  0.000130 

10.0 0.000335  0.000081 

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.010909  0.150781 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.006545  0.047538 

4.2    

4.5    

5.0 0.003682  0.012729 

6.0 0.002086  0.003465 

7.0 0.001202  0.001096 

8.0 0.000719  0.000462 

9.0 0.000450  0.000257 

10.0 0.000296  0.000164 

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.008865  0.159885 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.005428  0.050396 

4.2    

4.5    

5.0 0.003069  0.013948 

6.0 0.001741  0.004039 

7.0 0.001005  0.001398 

8.0 0.000602  0.000636 

9.0 0.000377  0.000365 

10.0 0.000248  0.000236 

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.006718  0.167317 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.004183  0.052671 

4.2    

4.5    

5.0 0.002375  0.014916 

6.0 0.001348  0.004497 

7.0 0.000779  0.001641 

8.0 0.000467  0.000775 

9.0 0.000292  0.000452 

10.0 0.000192  0.000293 

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.004508  0.172806 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.002842  0.054322 

4.2    

4.5    

5.0 0.001618  0.015618 

6.0 0.000919  0.004830 

7.0 0.000531  0.001818 

8.0 0.000319  0.000878 

9.0 0.000200  0.000516 

10.0 0.000131  0.000335 

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.002262  0.176181 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0 0.001437  0.055323 

4.2    

4.5    

5.0 0.000819  0.016044 

6.0 0.000466  0.005032 

7.0 0.000269  0.001925 

8.0 0.000162  0.000940 

9.0 0.000101  0.000555 

10.0 0.000067  0.000361 

R (a.u.),  = 90° Y† Y Z†Z

3.0   0.177316 

3.4    

3.5    

3.6    

3.7    

3.8    

3.9    

4.0   0.055659 

4.2    

4.5    

5.0   0.016187 

6.0   0.005100 

7.0   0.001961 

8.0   0.000961 

9.0   0.000569 

10.0   0.000370 

**Table S6.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 1.787 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.024249 

3.4  0  0.016660

3.5  0  0.012493

3.6  0  0.008359

3.7  0  0.004505

3.8  0  0.001076

3.9  0  0.001862

4.0 0 0 0.004298 0.004298

4.2  0  0.007784

4.5  0  0.010297

5.0 0 0 0.010436 0.010452

6.0 0 0 0.006866 0.006867

7.0 0 0 0.004014 0.004013

8.0 0 0 0.002373 0.002372

9.0 0 0 0.001461 0.001459

10.0 0 0 0.000946 0.000982

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.004026  0.024882 

3.4  0.003295  0.017281

3.5  0.003054  0.013110

3.6  0.002821  0.008967

3.7  0.002600  0.005100

3.8  0.002397  0.001654

3.9  0.002212  0.001305

4.0 0.002045 0.002045 0.003767 0.003767

4.2  0.001760  0.007309

4.5  0.001429  0.009911

5.0 0.001045 0.001045 0.010177 0.010192

6.0 0.000588 0.000588 0.006753 0.006755

7.0 0.000339 0.000339 0.003960 0.003960

8.0 0.000202 0.000202 0.002344 0.002343

9.0 0.000126 0.000126 0.001444 0.001442

10.0 0.000082 0.000050 0.000936 0.000971

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.007819  0.026829 

3.4  0.006409  0.019154

3.5  0.005945  0.014961

3.6  0.005494  0.010786

3.7  0.005069  0.006876

3.8  0.004677  0.003374

3.9  0.004319  0.000347

4.0 0.003996 0.003996 0.002191 0.002191

4.2  0.003443  0.005904

4.5  0.002800  0.008769

5.0 0.002049 0.002049 0.009412 0.009427

6.0 0.001154 0.001154 0.006420 0.006419

7.0 0.000666 0.000666 0.003801 0.003800

8.0 0.000396 0.000396 0.002257 0.002257

9.0 0.000247 0.000247 0.001393 0.001391

10.0 0.000161 0.000167 0.000903 0.000939

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.011165  0.030220 

3.4  0.009177  0.022300

3.5  0.008523  0.018047

3.6  0.007888  0.013800

3.7  0.007288  0.009801

3.8  0.006734  0.006193

3.9  0.006227  0.003045

4.0 0.005769 0.005769 0.000375 0.000375

4.2  0.004982  0.003624

4.5  0.004061  0.006924

5.0 0.002978 0.002978 0.008177 0.008193

6.0 0.001679 0.001679 0.005881 0.005880

7.0 0.000969 0.000969 0.003543 0.003542

8.0 0.000577 0.000577 0.002118 0.002117

9.0 0.000359 0.000359 0.001310 0.001308

10.0 0.000234 0.000242 0.000850 0.000886

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.013884  0.035238 

3.4  0.011467  0.026736

3.5  0.010669  0.022354

3.6  0.009893  0.017968

3.7  0.009159  0.013815

3.8  0.008479  0.010039

3.9  0.007857  0.006708

4.0 0.007291 0.007291 0.003843 0.003843

4.2  0.006315  0.000562

4.5  0.005165  0.004457

5.0 0.003799 0.003808 0.006532 0.006581

6.0 0.002144 0.002144 0.005161 0.005160

7.0 0.001238 0.001238 0.003196 0.003196

8.0 0.000737 0.000737 0.001929 0.001929

9.0 0.000459 0.000459 0.001198 0.001204

10.0 0.000300 0.000308 0.000778 0.000814

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.015856  0.042065 

3.4  0.013193  0.032444

3.5  0.012305  0.027830

3.6  0.011438  0.023213

3.7  0.010616  0.018821

3.8  0.009852  0.014798

3.9  0.009151  0.011213

4.0 0.008511 0.008511 0.008089 0.008087

4.2  0.007400  0.003160

4.5  0.006077  0.001477

5.0 0.004486 0.004486 0.004550 0.004580

6.0 0.002537 0.002537 0.004291 0.004290

7.0 0.001465 0.001465 0.002771 0.002775

8.0 0.000873 0.000873 0.001699 0.001699

9.0 0.000544 0.000544 0.001061 0.001067

10.0 0.000355 0.000365 0.000690 0.000725

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.017027  0.050826 

3.4  0.014316  0.039344

3.5  0.013393  0.034367

3.6  0.012488  0.029405

3.7  0.011627  0.024678

3.8  0.010822  0.020323

3.9  0.010079  0.016408

4.0 0.009398 0.009398 0.012957 0.012956

4.2  0.008207  0.007394

4.5  0.006772  0.001891

5.0 0.005020 0.005020 0.002317 0.002286

6.0 0.002845 0.002845 0.003307 0.003307

7.0 0.001644 0.001643 0.002296 0.002295

8.0 0.000980 0.000980 0.001436 0.001436

9.0 0.000612 0.000611 0.000903 0.000909

10.0 0.000400 0.000435 0.000589 0.000623

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.017409  0.061527 

3.4  0.014848  0.047281

3.5  0.013941  0.041796

3.6  0.013046  0.036365

3.7  0.012188  0.031199

3.8  0.011382 0.026424

3.9  0.010634  0.022106

4.0 0.009943 0.009943 0.018269 0.018267

4.2  0.008723  0.011978

4.5  0.007233  0.005498

5.0 0.005387 0.005387 0.000074 0.000064

6.0 0.003061 0.003061 0.002249 0.002251

7.0 0.001769 0.001769 0.001776 0.001775

8.0 0.001056 0.001056 0.001149 0.001149

9.0 0.000659 0.000658 0.000730 0.000736

10.0 0.000431 0.000465 0.000478 0.000511

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.017074  0.074020 

3.4  0.014830  0.056031

3.5  0.013985  0.049891

3.6  0.013141  0.043866

3.7  0.012324  0.038163

3.8  0.011550  0.032887

3.9  0.010825  0.028104

4.0 0.010152 0.010151 0.023829 0.023828

4.2  0.008950  0.016739

4.5  0.007460  0.009251

5.0 0.005581 0.005580 0.002535 0.002535

6.0 0.003180 0.003179 0.001154 0.001153

7.0 0.001839 0.001839 0.001233 0.001233

8.0 0.001099 0.001098 0.000848 0.000848

9.0 0.000687 0.000685 0.000548 0.000529

10.0 0.000449 0.000483 0.000360 0.000394

R (a. u.),  = 45° Y† Y Z†Z

3.0 0.016139  0.087965 

3.4  0.014341  0.065261

3.5  0.013585  0.058359

3.6  0.012812  0.051640

3.7  0.012073  0.045320

3.8  0.011357  0.039481

3.9  0.010680  0.034188

4.0 0.010044 0.010044 0.029442 0.029441

4.2  0.008898  0.021510

4.5  0.007454  0.012974

5.0 0.005601 0.005601 0.004979 0.004979

6.0 0.003200 0.003200 0.000059 0.000059

7.0 0.001853 0.001853 0.000687 0.000687

8.0 0.001108 0.001108 0.000543 0.000543

9.0 0.000693 0.000692 0.000362 0.000342

10.0 0.000454 0.000488 0.000240 0.000218

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.014747  0.102879 

3.4  0.013456  0.074676

3.5  0.012811  0.066854

3.6  0.012145  0.059399

3.7  0.011484  0.052411

3.8  0.010842  0.045982

3.9  0.010229  0.040151

4.0 0.009648 0.009648 0.034919 0.034918

4.2  0.008587  0.026136

4.5  0.007228  0.016563

5.0 0.005453 0.005453 0.007332 0.007332

6.0 0.003124 0.003124 0.001001 0.001001

7.0 0.001811 0.001811 0.000153 0.000152

8.0 0.001084 0.001084 0.000243 0.000243

9.0 0.000679 0.000668 0.000178 0.000158

10.0 0.000445 0.000415 0.000121 0.000101

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.013043  0.118152 

3.4  0.012259  0.083884

3.5  0.011731  0.075136

3.6  0.011172  0.066876

3.7  0.010606  0.059200

3.8  0.010049  0.052169

3.9  0.009510  0.045802

4.0 0.008994 0.008994 0.040090 0.040089

4.2  0.008039  0.030478

4.5  0.006796  0.019918

5.0 0.005147 0.005147 0.009528 0.009528

6.0 0.002956 0.002956 0.001998 0.001998

7.0 0.001715 0.001715 0.000354 0.000354

8.0 0.001028 0.001028 0.000043 0.000043

9.0 0.000644 0.000633 0.000003 0.000018

10.0 0.000423 0.000392 0.000006 0.000012

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.011162  0.133086 

3.4  0.010826  0.092550

3.5  0.010411  0.082868

3.6  0.009958  0.073820

3.7  0.009490  0.065471

3.8  0.009021  0.057857

3.9  0.008561  0.050979

4.0 0.008116 0.008116 0.044810 0.044810

4.2  0.007282  0.034424

4.5  0.006180  0.022954

5.0 0.004695 0.004696 0.011514 0.011514

6.0 0.002702 0.002702 0.002905 0.002905

7.0 0.001571 0.001571 0.000819 0.000819

8.0 0.000942 0.000942 0.000307 0.000307

9.0 0.000591 0.000579 0.000160 0.000182

10.0 0.000388 0.000357 0.000100 0.000115

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.009210  0.147017 

3.4  0.009220  0.100369

3.5  0.008908  0.089802

3.6  0.008554  0.080014

3.7  0.008180  0.071042

3.8  0.007798  0.062891

3.9  0.007419  0.055544

4.0 0.007048 0.007048 0.048963 0.048963

4.2  0.006345  0.037882

4.5  0.005402  0.025606

5.0 0.004116 0.004116 0.013249 0.013249

6.0 0.002373 0.002373 0.003703 0.003703

7.0 0.001381 0.001381 0.001231 0.001231

8.0 0.000829 0.000829 0.000542 0.000542

9.0 0.000520 0.000536 0.000306 0.000327

10.0 0.000342 0.000311 0.000196 0.000208

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.007265  0.159298 

3.4  0.007492  0.107083

3.5  0.007268  0.095730

3.6  0.007004  0.085289

3.7  0.006716  0.075766

3.8  0.006418  0.067146

3.9  0.006119  0.059396

4.0 0.005824 0.005824 0.052459 0.052459

4.2  0.005257  0.040784

4.5  0.004488  0.027826

5.0 0.003427 0.003427 0.014702 0.014702

6.0 0.001979 0.001979 0.004375 0.004375

7.0 0.001153 0.001153 0.001580 0.001581

8.0 0.000693 0.000693 0.000742 0.000742

9.0 0.000435 0.000452 0.000430 0.000451

10.0 0.000286 0.000255 0.000277 0.000289

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.005367  0.169415 

3.4  0.005680  0.112494

3.5  0.005529  0.100489

3.6  0.005343  0.089508

3.7  0.005135  0.079536

3.8  0.004917  0.070536

3.9  0.004696  0.062456

4.0 0.004475 0.004475 0.055233 0.055233

4.2  0.004048  0.043081

4.5  0.003463  0.029580

5.0 0.002649 0.002649 0.015851 0.015851

6.0 0.001532 0.001532 0.004909 0.004909

7.0 0.000893 0.000893 0.001860 0.001860

8.0 0.000537 0.000537 0.000903 0.000903

9.0 0.000338 0.000355 0.000530 0.000551

10.0 0.000222 0.000191 0.000343 0.000354

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.003532  0.176931 

3.4  0.003814  0.116454

3.5  0.003722  0.103963

3.6  0.003603  0.092582

3.7  0.003469  0.082276

3.8  0.003327  0.072996

3.9  0.003181  0.064675

4.0 0.003034 0.003034 0.057241 0.057241

4.2  0.002749  0.044742

4.5  0.002355  0.030856

5.0 0.001804 0.001804 0.016681 0.016681

6.0 0.001044 0.001044 0.005297 0.005297

7.0 0.000609 0.000609 0.002063 0.002063

8.0 0.000367 0.000367 0.001020 0.001020

9.0 0.000230 0.000249 0.000604 0.000623

10.0 0.000152 0.000120 0.000392 0.000402

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.001751  0.181565 

3.4  0.001915  0.118866

3.5  0.001871  0.106075

3.6  0.001814  0.094449

3.7  0.001748  0.083939

3.8  0.001678  0.074486

3.9  0.001605  0.066017

4.0 0.001532 0.001532 0.058455 0.058455

4.2  0.001389  0.045745

4.5  0.001191  0.031611

5.0 0.000913 0.000913 0.017182 0.017183

6.0 0.000529 0.000529 0.005531 0.005531

7.0 0.000309 0.000309 0.002187 0.002187

8.0 0.000186 0.000186 0.001091 0.001091

9.0 0.000117 0.000136 0.000648 0.000668

10.0 0.000077 0.000045 0.000421 0.000424

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.183115 

3.4  0  0.119670

3.5  0  0.106778

3.6  0  0.095070

3.7  0  0.084493

3.8  0  0.074983

3.9  0  0.066465

4.0 0 0 0.058862 0.058861

4.2  0  0.046079

4.5  0  0.031867

5.0 0 0 0.017350 0.017350

6.0 0 0 0.005610 0.005610

7.0 0 0 0.002228 0.002228

8.0 0 0 0.001116 0.001116

9.0 0 0 0.000663 0.000682

10.0 0 0 0.000431 0.000434

**Table S7.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 2.125 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.009852 

3.4  0  0.000583

3.5  0  0.002094

3.6  0  0.005561

3.7  0  0.009433

3.8  0  0.013181

3.9  0  0.016568

4.0 0 0 0.019202 0.019194

4.2  0  0.022672

4.5  0  0.023639

5.0 0 0 0.019811 0.019821

6.0 0 0 0.010524 0.010542

7.0 0 0 0.005467 0.005467

8.0 0 0 0.003056 0.003055

9.0 0 0 0.001840 0.001839

10.0 0 0 0.001182 0.001101

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.003999  0.009885 

3.4  0.004241  0.000780

3.5  0.004050  0.001816

3.6  0.003807  0.005212

3.7  0.003535  0.009012

3.8  0.003256  0.012698

3.9  0.003056  0.016034

4.0 0.002728 0.002728 0.018637 0.018628

4.2  0.002285  0.022013

4.5  0.001788  0.023097

5.0 0.001270 0.001264 0.019420 0.019431

6.0 0.000724 0.000724 0.010357 0.010357

7.0 0.000426 0.000426 0.005392 0.005391

8.0 0.000255 0.000255 0.003017 0.003016

9.0 0.000159 0.000159 0.001818 0.001816

10.0 0.000103 0.000129 0.001168 0.001089

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.007678  0.009869 

3.4  0.008174  0.001480

3.5  0.007808  0.000887

3.6  0.007342  0.004095

3.7  0.006824  0.007698

3.8  0.006292  0.011213

3.9  0.005842  0.014344

4.0 0.005285 0.005285 0.016932 0.016925

4.2  0.004439  0.020278

4.5  0.003488  0.021485

5.0 0.002488 0.002487 0.018270 0.018280

6.0 0.001420 0.001420 0.009866 0.009866

7.0 0.000836 0.000835 0.005170 0.005170

8.0 0.000501 0.000501 0.002902 0.002901

9.0 0.000312 0.000312 0.001751 0.001750

10.0 0.000203 0.000234 0.001126 0.001049

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.010734  0.009471 

3.4  0.011520  0.002938

3.5  0.011013  0.000937

3.6  0.010367  0.002033

3.7  0.009649  0.005354

3.8  0.008912  0.008634

3.9  0.008194  0.011591

4.0 0.007521 0.007521 0.014071 0.014064

4.2  0.006347  0.017389

4.5  0.005019  0.018893

5.0 0.003604 0.003602 0.016420 0.016429

6.0 0.002064 0.002064 0.009075 0.009075

7.0 0.001215 0.001215 0.004812 0.004811

8.0 0.000728 0.000728 0.002716 0.002715

9.0 0.000454 0.000454 0.001643 0.001642

10.0 0.000295 0.000303 0.001058 0.000981

R (a.u.),  = 20° Y Y Z Z

3.0 0.012912  0.008155 

3.4  0.014061  0.005532

3.5  0.013464  0.003865

3.6  0.012699  0.001226

3.7  0.011848  0.001802

3.8  0.010910  0.004794

3.9  0.010122  0.007650

4.0 0.009322 0.009321 0.010053 0.010046

4.2  0.007912  0.013440

4.5  0.006320  0.015402

5.0 0.004579 0.004580 0.013965 0.013973

6.0 0.002634 0.002634 0.008026 0.008004

7.0 0.001551 0.001551 0.004333 0.004333

8.0 0.000930 0.000930 0.002466 0.002465

9.0 0.000580 0.000580 0.001498 0.001497

10.0 0.000377 0.000381 0.000966 0.000888

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.014048  0.005193 

3.4  0.015671  0.009680

3.5  0.015122  0.008401

3.6  0.014239  0.005917

3.7  0.013355  0.003104

3.8  0.012400  0.000213

3.9  0.011488  0.002512

4.0 0.010627 0.010627 0.004921 0.004969

4.2  0.009121  0.008539

4.5  0.007346  0.011159

5.0 0.005379 0.005380 0.011033 0.011033

6.0 0.003111 0.003111 0.006770 0.006759

7.0 0.001832 0.001833 0.003757 0.003757

8.0 0.001101 0.001101 0.002163 0.002162

9.0 0.000687 0.000687 0.001321 0.001320

10.0 0.000447 0.000446 0.000854 0.000775

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.014074  0.000458 

3.4  0.016315  0.015731

3.5  0.015750  0.014440

3.6  0.015082  0.012187

3.7  0.014100  0.009400

3.8  0.013184  0.006504

3.9  0.012165  0.003749

4.0 0.011426 0.011426 0.001208 0.001232

4.2  0.009897  0.002842

4.5  0.008083  0.006364

5.0 0.005986 0.005986 0.007744 0.007748

6.0 0.003481 0.003481 0.005366 0.005367

7.0 0.002052 0.002052 0.003107 0.003116

8.0 0.001234 0.001234 0.001819 0.001818

9.0 0.000770 0.000763 0.001119 0.001117

10.0 0.000502 0.000498 0.000725 0.000646

R (a.u.), = 35° Y† Y Z†Z

3.0 0.012955  0.008942 

3.4  0.016072  0.023867

3.5  0.015637  0.022431

3.6  0.014917  0.019959

3.7  0.014205  0.017099

3.8  0.013380  0.014000

3.9  0.012547  0.010981

4.0 0.011748 0.011748 0.008143 0.008136

4.2  0.010296  0.003432

4.5  0.008521  0.001197

5.0 0.006386 0.006387 0.004261 0.004262

6.0 0.003737 0.003737 0.003875 0.003875

7.0 0.002205 0.002205 0.002409 0.002408

8.0 0.001327 0.001327 0.001446 0.001445

9.0 0.000830 0.000820 0.000898 0.000896

10.0 0.000541 0.000550 0.000584 0.000505

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.010891  0.020936 

3.4  0.015103  0.034028

3.5  0.014858  0.032099

3.6  0.014379  0.029231

3.7  0.013759  0.025844

3.8  0.013068  0.022389

3.9  0.012355  0.018867

4.0 0.011652 0.011652 0.015619 0.015614

4.2  0.010340  0.010032

4.5  0.008675  0.004142

5.0 0.006579 0.006580 0.000719 0.000715

6.0 0.003872 0.003872 0.002353 0.002354

7.0 0.002287 0.002287 0.001689 0.001689

8.0 0.001378 0.001378 0.001058 0.001057

9.0 0.000862 0.000849 0.000666 0.000665

10.0 0.000564 0.000574 0.000436 0.000353

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.008185  0.036750 

3.4  0.013609  0.045884

3.5  0.013595  0.043085

3.6  0.013326  0.039440

3.7  0.012893  0.035377

3.8  0.012365  0.031202

3.9  0.011793  0.027142

4.0 0.011209 0.011209 0.023332 0.023328

4.2  0.010074  0.016700

4.5  0.008565  0.009406

5.0 0.006569 0.006569 0.002756 0.002764

6.0 0.003888 0.003888 0.000854 0.000855

7.0 0.002298 0.002298 0.000972 0.000971

8.0 0.001386 0.001386 0.000675 0.000667

9.0 0.000869 0.000849 0.000432 0.000427

10.0 0.000569 0.000584 0.000285 0.000197

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.005198  0.056091 

3.4  0.011814  0.058877

3.5  0.012036  0.054860

3.6  0.011978  0.050165

3.7  0.011735  0.045183

3.8  0.011376  0.040210

3.9  0.010949  0.035431

4.0 0.010488 0.010488 0.030968 0.030964

4.2  0.009544  0.023186

4.5  0.008215  0.014462

5.0 0.006365 0.006366 0.006053 0.006034

6.0 0.003786 0.003786 0.000576 0.000576

7.0 0.002240 0.002240 0.000279 0.000278

8.0 0.001353 0.001353 0.000287 0.000286

9.0 0.000849 0.000821 0.000201 0.000197

10.0 0.000556 0.000565 0.000136 0.000042

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.002309  0.078137 

3.4  0.009914  0.072304

3.5  0.010338  0.066810

3.6  0.010468  0.060867

3.7  0.010396  0.054836

3.8  0.010189  0.048959

3.9  0.009895  0.043393

4.0 0.009551 0.009551 0.038235 0.038232

4.2  0.008793  0.029271

4.5  0.007655  0.019144

5.0 0.005983 0.005983 0.009085 0.009089

6.0 0.003574 0.003574 0.001900 0.001900

7.0 0.002117 0.002117 0.000371 0.000372

8.0 0.001280 0.001280 0.000073 0.000074

9.0 0.000805 0.000804 0.000018 0.000023

10.0 0.000528 0.000534 0.000006 0.000101

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.000140  0.101632 

3.4  0.008058  0.085426

3.5  0.008626  0.078314

3.6  0.008897  0.071043

3.7  0.008957  0.063906

3.8  0.008873  0.057097

3.9  0.008691  0.050735

4.0 0.008448 0.008447 0.044886 0.044883

4.2  0.007859  0.034727

4.5  0.006907  0.023338

5.0 0.005439 0.005439 0.011787 0.011784

6.0 0.003261 0.003261 0.003090 0.003090

7.0 0.001934 0.001934 0.000961 0.000962

8.0 0.001171 0.001170 0.000403 0.000404

9.0 0.000737 0.000704 0.000220 0.000225

10.0 0.000484 0.000486 0.000138 0.000230

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.001899  0.124988 

3.4  0.006334  0.097557

3.5  0.006974  0.088829

3.6  0.007326  0.080247

3.7  0.007473  0.072036

3.8  0.007475  0.064335

3.9  0.007379  0.057221

4.0 0.007216 0.007215 0.050728 0.050726

4.2  0.006773  0.039572

4.5  0.006000  0.026962

5.0 0.004754 0.004754 0.014114 0.014111

6.0 0.002858 0.002858 0.004122 0.004122

7.0 0.001698 0.001698 0.001480 0.001481

8.0 0.001029 0.001028 0.000695 0.000695

9.0 0.000648 0.000633 0.000400 0.000404

10.0 0.000426 0.000424 0.000255 0.000343

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.002843  0.146621 

3.4  0.004788  0.108132

3.5  0.005418  0.097912

3.6  0.005810  0.088136

3.7  0.005924  0.079010

3.8  0.006011  0.070463

3.9  0.005951  0.062705

4.0 0.005885 0.005964 0.055627 0.055637

4.2  0.005550  0.043603

4.5  0.004961  0.029963

5.0 0.003949 0.003949 0.016036 0.016034

6.0 0.002380 0.002380 0.004981 0.004982

7.0 0.001415 0.001415 0.001916 0.001917

8.0 0.000858 0.000858 0.000942 0.000942

9.0 0.000541 0.000537 0.000553 0.000510

10.0 0.000356 0.000351 0.000356 0.000437

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.002976  0.165036 

3.4  0.003482  0.116722

3.5  0.003961  0.105240

3.6  0.004294  0.094465

3.7  0.004474  0.084483

3.8  0.004545  0.075331

3.9  0.004505  0.067065

4.0 0.004478 0.004478 0.059495 0.059492

4.2  0.004257  0.046702

4.5  0.003814  0.032312

5.0 0.003047 0.003047 0.017540 0.017538

6.0 0.001839 0.001839 0.005658 0.005635

7.0 0.001095 0.001095 0.002261 0.002263

8.0 0.000664 0.000664 0.001139 0.001139

9.0 0.000419 0.000419 0.000675 0.000624

10.0 0.000276 0.000269 0.000437 0.000510

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.002410  0.179037 

3.4  0.002191  0.123033

3.5  0.002590  0.110600

3.6  0.002839  0.099075

3.7  0.002979  0.088495

3.8  0.002922  0.078914

3.9  0.003048  0.070153

4.0 0.003016 0.003016 0.062281 0.062278

4.2  0.002878  0.048951

4.5  0.002587  0.033994

5.0 0.002072 0.002072 0.018616 0.018590

6.0 0.001252 0.001252 0.006144 0.006173

7.0 0.000746 0.000746 0.002512 0.002513

8.0 0.000453 0.000453 0.001282 0.001283

9.0 0.000286 0.000288 0.000764 0.000706

10.0 0.000188 0.000182 0.000496 0.000421

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.001337  0.187777 

3.4  0.001069  0.126884

3.5  0.001279  0.113860

3.6  0.001412  0.101872

3.7  0.001488  0.090979

3.8  0.001524  0.080985

3.9  0.001530  0.072016

4.0 0.001517 0.001517 0.063960 0.063957

4.2  0.001451  0.050299

4.5  0.001323  0.035022

5.0 0.001048 0.001048 0.019262 0.019264

6.0 0.000634 0.000634 0.006437 0.006439

7.0 0.000378 0.000378 0.002663 0.002664

8.0 0.000230 0.000229 0.001369 0.001370

9.0 0.000145 0.000148 0.000819 0.000754

10.0 0.000096 0.000092 0.000532 0.000456

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.190741 

3.4  0  0.128180

3.5  0  0.114956

3.6  0  0.102815

3.7  0  0.091740

3.8  0  0.081703

3.9  0  0.072650

4.0 0 0 0.064526 0.064522

4.2  0  0.050770

4.5  0  0.035345

5.0 0 0 0.019478 0.019477

6.0 0 0 0.006535 0.006537

7.0 0 0 0.002714 0.002715

8.0 0 0 0.001398 0.001399

9.0 0 0 0.000837 0.000771

10.0 0 0 0.000544 0.000468

**Table S8.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 2.463 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.020142 

3.4  0  0.003842

3.5  0  0.004446

3.6  0  

3.7  0  0.000057

3.8  0  

3.9  0  0.010361

4.0 0 0 0.016118 0.016107

4.2  0  0.025711

4.5  0  0.032660

5.0 0 0 0.029205 0.029211

6.0 0 0 0.014509 0.014503

7.0 0 0 0.006909 0.006915

8.0 0 0 0.003658 0.003660

9.0 0 0 0.002149 0.002136

10.0 0 0 0.001367 0.001344

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.003208  0.020815 

3.4  0.004597  0.003275

3.5  0.004472  0.003720

3.6    

3.7  0.004581  0.000512

3.8    

3.9  0.004072  0.010507

4.0 0.003766 0.003766 0.016116 0.016112

4.2  0.003122  0.025387

4.5  0.002300  0.032108

5.0 0.001487 0.001488 0.028699 0.028662

6.0 0.000820 0.000912 0.014278 0.014279

7.0 0.000492 0.000492 0.006810 0.006817

8.0 0.000298 0.000298 0.003609 0.003611

9.0 0.000186 0.000189 0.002122 0.002109

10.0 0.000121 0.000434 0.001350 0.001327

R (a.u.), = 10° Y† Y Z†Z

3.0 0.006041  0.022744 

3.4  0.008808  0.001723

3.5  0.008975  0.002233

3.6    

3.7  0.008749  0.001016

3.8  0.008318  0.005477

3.9  0.007799  0.010801

4.0 0.007213 0.007212 0.015996 0.015340

4.2  0.006048  0.024550

4.5  0.004438  0.030261

5.0 0.002898 0.002898 0.027204 0.027168

6.0 0.001608 0.001609 0.013598 0.013599

7.0 0.000965 0.000965 0.006519 0.006525

8.0 0.000584 0.000585 0.003467 0.003468

9.0 0.000365 0.000369 0.002042 0.002029

10.0 0.000237 0.000520 0.001300 0.001277

R (a.u.), = 15° Y† Y Z†Z

3.0 0.008132  0.025665 

3.4  0.012270  0.000242

3.5  0.012523  0.000514

3.6  0.012533  

3.7    

3.8  0.011607  0.006118

3.9  0.010884  0.010324

4.0 0.010067 0.010069 0.015443 0.015467

4.2  0.008389  0.022857

4.5  0.006277  0.027847

5.0 0.004163 0.004163 0.024792 0.024757

6.0 0.002335 0.002335 0.012510 0.012512

7.0 0.001402 0.001402 0.006051 0.006057

8.0 0.000850 0.000850 0.003235 0.003236

9.0 0.000531 0.000535 0.001911 0.001899

10.0 0.000344 0.000544 0.001220 0.001066

R (a.u.), = 20° Y† Y Z†Z

3.0 0.009152  0.029111 

3.4  0.014675  0.002829

3.5    

3.6  0.014951  0.001256

3.7    

3.8  0.013691  0.006759

3.9  0.013102  0.010326

4.0 0.012133 0.012140 0.014020 0.013999

4.2  0.010176  0.020120

4.5  0.007722  0.024121

5.0 0.005232 0.005187 0.021578 0.021536

6.0 0.002974 0.002973 0.011079 0.011094

7.0 0.001787 0.001785 0.005432 0.005437

8.0 0.001084 0.001085 0.002927 0.002928

9.0 0.000678 0.000683 0.001737 0.001724

10.0 0.000440 0.000553 0.001111 0.000957

R (a.u.), = 25° Y† Y Z†Z

3.0 0.008829  0.032396 

3.4  0.015792  0.004350

3.5  0.016365  

3.6    

3.7  0.015929  0.002859

3.8  0.015237  0.005882

3.9  0.014341  0.007906

4.0 0.013326 0.013335 0.011284 0.011263

4.2  0.011290  0.016255

4.5  0.008733  0.019565

5.0 0.006073 0.006070 0.017720 0.017711

6.0 0.003505 0.003504 0.009384 0.009304

7.0 0.002109 0.002107 0.004692 0.004697

8.0 0.001281 0.001281 0.002556 0.002557

9.0 0.000801 0.000807 0.001525 0.001379

10.0 0.000521 0.000582 0.000978 0.000825

R (a.u.), = 30° Y† Y Z†Z

3.0 0.006984  0.034595 

3.4    

3.5    

3.6  0.016345  0.000227

3.7  0.016038  0.001056

3.8  0.015581  0.002215

3.9  0.014619  0.004602

4.0 0.013677 0.013681 0.006922 0.006900

4.2  0.011761  0.010917

4.5  0.009321  0.013986

5.0 0.006671 0.006667 0.013404 0.013380

6.0 0.003913 0.003896 0.007512 0.007478

7.0 0.002358 0.002348 0.003867 0.003858

8.0 0.001433 0.001434 0.002137 0.002138

9.0 0.000897 0.000906 0.001284 0.001139

10.0 0.000584 0.000617 0.000827 0.000673

R (a.u.), = 35° Y† Y Z†Z

3.0 0.003564  0.034549 

3.4  0.014011  

3.5  0.014890  0.002612

3.6  0.015239  0.004020

3.7  0.015158  0.003552

3.8  0.014735  0.002752

3.9  0.014089  0.001280

4.0 0.013315 0.013198 0.000852 0.000983

4.2  0.011846  0.004548

4.5  0.009530  0.007817

5.0 0.007030 0.007027 0.008832 0.008871

6.0 0.004190 0.004187 0.005550 0.005548

7.0 0.002528 0.002528 0.002992 0.002992

8.0 0.001538 0.001537 0.001687 0.001688

9.0 0.000964 0.000975 0.001023 0.000878

10.0 0.000629 0.000647 0.000662 0.000654

R (a.u.), = 40° Y† Y Z†Z

3.0 0.001311  0.030923 

3.4  0.011326  0.006111

3.5  0.012672  0.009270

3.6  0.013276  0.011353

3.7  0.013487  0.011092

3.8  0.013271  0.010407

3.9  0.012981  0.008816

4.0 0.012429 0.012420 0.006734 0.006740

4.2  0.011196  0.003021

4.5  0.009419  0.001258

5.0 0.007160 0.007157 0.004204 0.004119

6.0 0.004330 0.004328 0.003579 0.003576

7.0 0.002616 0.002616 0.002102 0.002102

8.0 0.001593 0.001592 0.001223 0.001214

9.0 0.001000 0.001015 0.000752 0.000752

10.0 0.000653 0.000663 0.000489 0.000515

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.007308  0.022340 

3.4  0.007997  0.016544

3.5  0.009482  0.019556

3.6  0.011004  0.020883

3.7  0.011380  0.020759

3.8  0.011540  0.019839

3.9  0.011483  0.017665

4.0 0.011219 0.011284 0.015410 0.015109

4.2  0.010385  0.010877

4.5  0.009132  0.005305

5.0 0.007078 0.006988 0.000298 0.000158

6.0 0.004336 0.004334 0.001671 0.001667

7.0 0.002622 0.002622 0.001226 0.001226

8.0 0.001599 0.001731 0.000760 0.000625

9.0 0.001005 0.000987 0.000478 0.000515

10.0 0.000658 0.000676 0.000315 0.000340

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.013846  0.007644 

3.4  0.004507  0.030640

3.5  0.007276  0.032878

3.6  0.008247  0.033367

3.7  0.009164  0.032275

3.8  0.009740  0.030256

3.9  0.009868  0.027497

4.0 0.009858 0.009892 0.024615 0.024689

4.2  0.009708  0.018998

4.5  0.008483  0.011715

5.0 0.006802 0.006844 0.004523 0.004605

6.0 0.004212 0.004210 0.000119 0.000124

7.0 0.002550 0.002549 0.000392 0.000393

8.0 0.001556 0.001690 0.000314 0.000177

9.0 0.000980 0.001009 0.000211 0.000248

10.0 0.000642 0.000664 0.000143 0.000169

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.019939  0.014488 

3.4  0.001372  0.045763

3.5  0.004007  0.048290

3.6  0.005680  0.046967

3.7  0.007321  0.044779

3.8  0.007842  0.041254

3.9  0.008205  0.037412

4.0 0.008468 0.008536 0.033767 0.033659

4.2  0.008440  0.026473

4.5  0.007702  0.017612

5.0 0.006351 0.006354 0.008359 0.008341

6.0 0.003968 0.003966 0.001747 0.001631

7.0 0.002404 0.002405 0.000379 0.000378

8.0 0.001468 0.001604 0.000105 0.000069

9.0 0.000927 0.000970 0.000041 0.000004

10.0 0.000608 0.000637 0.000020 0.000034

R (a.u.), = 60° Y† Y Z†Z

3.0 0.024910  0.042350 

3.4  0.001131  0.065679

3.5  0.001748  0.064013

3.6  0.003809  0.060808

3.7  0.005355  0.056518

3.8  0.006282  0.051879

3.9  0.006699  0.047141

4.0 0.007116 0.007113 0.042353 0.042367

4.2  0.007285  0.033534

4.5  0.006893  0.022842

5.0 0.005744 0.005757 0.011727 0.011912

6.0 0.003613 0.003609 0.003185 0.003181

7.0 0.002191 0.002192 0.001072 0.001071

8.0 0.001340 0.001339 0.000486 0.000449

9.0 0.000847 0.000845 0.000272 0.000275

10.0 0.000557 0.000573 0.000170 0.000184

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.027636  0.074934 

3.4  0.002718  0.083635

3.5  0.000195  0.079268

3.6  0.002288  0.073847

3.7  0.003759  0.067888

3.8  0.004762  0.061769

3.9  0.005420  0.055748

4.0 0.005827 0.005824 0.049986 0.049997

4.2  0.006132  0.039655

4.5  0.005919  0.027420

5.0 0.005002 0.004997 0.014584 0.014511

6.0 0.003162 0.003161 0.004413 0.004410

7.0 0.001919 0.001920 0.001672 0.001671

8.0 0.001174 0.001174 0.000818 0.000782

9.0 0.000743 0.000744 0.000476 0.000479

10.0 0.000489 0.000530 0.000303 0.000314

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.027469  0.109236 

3.4  0.003397  0.099934

3.5  0.000699  0.092844

3.6  0.001240  0.085270

3.7  0.002611  0.077613

3.8  0.003558  0.070146

3.9  0.004196  0.063040

4.0 0.004600 0.004599 0.056405 0.056409

4.2  0.004949  0.044737

4.5  0.004855  0.031156

5.0 0.004144 0.004139 0.016912 0.016890

6.0 0.002629 0.002629 0.005421 0.005420

7.0 0.001597 0.001598 0.002171 0.002171

8.0 0.000978 0.000978 0.001098 0.001061

9.0 0.000620 0.000621 0.000648 0.000652

10.0 0.000408 0.000474 0.000417 0.000422

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.024160  0.141464 

3.4  0.003272  0.113478

3.5  0.000953  0.103894

3.6  0.000593  0.094519

3.7  0.001736  0.085416

3.8  0.002701  0.076981

3.9  0.002924  0.068963

4.0 0.003418 0.003290 0.061463 0.061591

4.2  0.003742  0.048460

4.5  0.003714  0.034095

5.0 0.003191 0.003188 0.018708 0.018686

6.0 0.002029 0.002029 0.006205 0.006205

7.0 0.001234 0.001235 0.002564 0.002475

8.0 0.000756 0.000755 0.001319 0.001283

9.0 0.000479 0.000482 0.000786 0.000789

10.0 0.000316 0.000406 0.000508 0.000504

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.017958  0.167779 

3.4  0.002523  0.123543

3.5  0.000914  0.112151

3.6  0.000238  0.101289

3.7  0.001055  0.091098

3.8  0.001624  0.081654

3.9  0.002012  0.072945

4.0 0.002267 0.002267 0.065093 0.065123

4.2  0.002511  0.051647

4.5  0.002510  0.036296

5.0 0.002168 0.002165 0.019980 0.019889

6.0 0.001380 0.001381 0.006764 0.006761

7.0 0.000840 0.000841 0.002847 0.002756

8.0 0.000515 0.000515 0.001480 0.001482

9.0 0.000327 0.000329 0.000886 0.000889

10.0 0.000216 0.000212 0.000575 0.000559

R (a. u.),  = 85° Y† Y Z†Z

3.0 0.009565  0.184957 

3.4  0.001364  0.129714

3.5  0.000526  0.117141

3.6  0.000073  0.105394

3.7  0.000498  0.094582

3.8  0.000794  0.084563

3.9  0.000997  0.075487

4.0 0.001130 0.001131 0.067275 0.067271

4.2  0.001261  0.053073

4.5  0.001265  0.037297

5.0 0.001096 0.001094 0.020737 0.020750

6.0 0.000699 0.000698 0.007099 0.007096

7.0 0.000425 0.000426 0.003017 0.002926

8.0 0.000261 0.000261 0.001577 0.001579

9.0 0.000165 0.000168 0.000947 0.000950

10.0 0.000109 0.000144 0.000615 0.000590

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.190924 

3.4  0  0.131785

3.5  0  0.118808

3.6  0  0.106761

3.7  0  0.095669

3.8  0  0.085529

3.9  0  0.076318

4.0 0 0 0.067994 0.067993

4.2  0  0.053871

4.5  0  0.037729

5.0 0 0 0.020989 0.020980

6.0 0 0 0.007210 0.007207

7.0 0 0 0.003074 0.002983

8.0 0 0 0.001609 0.001612

9.0 0 0 0.000967 0.000971

10.0 0 0 0.000629 0.000599

**Table S9.** Dipole moments in the y and z directions for H2 ⋅ ⋅ ⋅ H with an H-H bond length r = 2.801 a.u., as a function of the angle  between the H2 bond axis and the pair-fixed Z axis and distance R from the H nucleus to the center of mass of H2. Results with aug-cc-pV5Z basis sets. † designates calculations with Molpro 2012 and tighter convergence criteria (see text).

R (a.u.),  = 0° Y† Y Z†Z

3.0 0  0.020077 

3.4  0  0.009469

3.5  0  0.014335

3.6  0  0.017813

3.7  0  0.019354

3.8  0  0.019083

3.9  0  0.016836

4.0 0 0 0.012679 0.012805

4.2  0  0.000199

4.5  0  0.021230

5.0 0 0 0.033170 0.033361

6.0 0 0 0.018166 0.018172

7.0 0 0 0.008144 0.008197

8.0 0 0 0.004089 0.004091

9.0 0 0 0.002337 0.002344

10.0 0 0 0.001469 0.001474

R (a.u.),  = 5° Y† Y Z†Z

3.0 0.002386  0.020915 

3.4  0.004062  0.008624

3.5  0.004350  0.013477

3.6  0.004573  0.016949

3.7  0.004725  0.018471

3.8  0.004794  0.018196

3.9  0.004775  0.015958

4.0 0.004664 0.004662 0.011835 0.011977

4.2  0.004118  0.000454

4.5  0.003207  0.021380

5.0 0.001830 0.001829 0.032730 0.032914

6.0 0.000870 0.000869 0.017870 0.017877

7.0 0.000526 0.000520 0.008021 0.008078

8.0 0.000322 0.000319 0.004032 0.004034

9.0 0.000202 0.000202 0.002306 0.002313

10.0 0.000131 0.000131 0.001450 0.001454

R (a.u.),  = 10° Y† Y Z†Z

3.0 0.004369  0.023387 

3.4  0.007745  0.006151

3.5  0.008319  0.010981

3.6  0.008761  0.014427

3.7  0.009057  0.015918

3.8  0.009189  0.015638

3.9  0.009147  0.014149

4.0 0.008919 0.008919 0.009437 0.009633

4.2  0.008135  0.002205

4.5  0.006110  0.021408

5.0 0.003521 0.003519 0.031400 0.031437

6.0 0.001704 0.001703 0.017003 0.017012

7.0 0.001031 0.001028 0.007661 0.007713

8.0 0.000632 0.000629 0.003864 0.003867

9.0 0.000396 0.000397 0.002215 0.002221

10.0 0.000257 0.000257 0.001395 0.001399

R (a.u.),  = 15° Y† Y Z†Z

3.0 0.005612  0.027361 

3.4  0.010678  0.002245

3.5  0.011535  0.007063

3.6  0.012195  0.010456

3.7  0.012626  0.011969

3.8  0.012926  0.011664

3.9  0.012732  0.009457

4.0 0.012351 0.012547 0.005009 0.005118

4.2  0.011176  0.004512

4.5  0.008522  0.021459

5.0 0.004959 0.004959 0.029164 0.029531

6.0 0.002467 0.002463 0.015623 0.015549

7.0 0.001497 0.001503 0.007086 0.007136

8.0 0.000918 0.000916 0.003595 0.003589

9.0 0.000576 0.000577 0.002069 0.002075

10.0 0.000373 0.000503 0.001306 0.001310

R (a.u.),  = 20° Y† Y Z†Z

3.0 0.005711  0.032591 

3.4  0.012578  0.002598

3.5  0.013658  0.002128

3.6  0.014529  0.005468

3.7  0.015088  0.006780

3.8  0.014948  0.007036

3.9  0.015191  0.005029

4.0 0.014837 0.014838 0.001555 0.001664

4.2  0.013279  0.007064

4.5  0.010116  0.021676

5.0 0.006075 0.006075 0.026029 0.025933

6.0 0.003131 0.003126 0.013818 0.013840

7.0 0.001907 0.001915 0.006331 0.006379

8.0 0.001171 0.001170 0.003239 0.003234

9.0 0.000734 0.000735 0.001873 0.001879

10.0 0.000475 0.000480 0.001186 0.001190

R (a.u.),  = 25° Y† Y Z†Z

3.0 0.004358  0.038693 

3.4  0.012968  0.008191

3.5  0.014399  0.003210

3.6  0.015481  0.000276

3.7  0.016162  0.001797

3.8  0.016436  0.001740

3.9  0.016517  0.000422

4.0 0.015000 0.015921 0.001605 0.001753

4.2  0.014177  0.008768

4.5  0.010927  0.019140

5.0 0.006848 0.006973 0.022069 0.021736

6.0 0.003676 0.003670 0.011698 0.011715

7.0 0.002247 0.002249 0.005439 0.005486

8.0 0.001380 0.001380 0.002812 0.002803

9.0 0.000866 0.000867 0.001637 0.001642

10.0 0.000563 0.000598 0.001041 0.001044

R (a.u.),  = 30° Y† Y Z†Z

3.0 0.001284  0.045102 

3.4  0.011813  0.013360

3.5  0.013551  0.007905

3.6  0.014861  0.004246

3.7  0.015697  0.001986

3.8  0.015973  0.002024

3.9  0.016221  0.001970

4.0 0.015858 0.015709 0.003251 0.003031

4.2  0.014135  0.009469

4.5  0.011074  0.015832

5.0 0.007296 0.007416 0.017437 0.017481

6.0 0.004087 0.004080 0.009382 0.009488

7.0 0.002507 0.002506 0.004457 0.004483

8.0 0.001542 0.001542 0.002336 0.002327

9.0 0.000968 0.000969 0.001371 0.001375

10.0 0.000630 0.000630 0.000875 0.000878

R (a.u.),  = 35° Y† Y Z†Z

3.0 0.003700  0.051034 

3.4  0.009204  0.017246

3.5  0.011036  0.010831

3.6  0.012647  0.007388

3.7  0.013679  0.005457

3.8  0.014530  0.002595

3.9  0.014910  0.001927

4.0 0.014456 0.014239 0.002249 0.002125

4.2  0.013176  0.006606

4.5  0.010693  0.011165

5.0 0.007464 0.007467 0.012357 0.012413

6.0 0.004358 0.004545 0.006987 0.007050

7.0 0.002682 0.002677 0.003429 0.003464

8.0 0.001651 0.001651 0.001830 0.001850

9.0 0.001038 0.001046 0.001084 0.001087

10.0 0.000677 0.000677 0.000696 0.000698

R (a.u.),  = 40° Y† Y Z†Z

3.0 0.010666  0.055438 

3.4  0.004450  0.017999

3.5  0.007044  0.011605

3.6  0.009161  0.003356

3.7  0.010795  0.002866

3.8  0.011773  0.000016

3.9  0.011813  0.001099

4.0 0.012179 0.011560 0.000142 0.001125

4.2  0.011633  0.001789

4.5  0.009828  0.004711

5.0 0.007401 0.007350 0.007094 0.007001

6.0 0.004488 0.004479 0.004620 0.004639

7.0 0.002769 0.002763 0.002400 0.002393

8.0 0.001706 0.001706 0.001313 0.001317

9.0 0.001074 0.001075 0.000788 0.000790

10.0 0.000702 0.000840 0.000510 0.000513

R (a.u.),  = 45° Y† Y Z†Z

3.0 0.019521  0.057004 

3.4  0.001257  0.015108

3.5  0.001931  0.007778

3.6  0.004702  0.001592

3.7  0.006711  0.003257

3.8  0.008138  0.005268

3.9  0.009130  0.006182

4.0 0.009693 0.009698 0.006549 0.007154

4.2  0.009620  0.004930

4.5  0.009009  0.001587

5.0 0.007152 0.007171 0.001910 0.001982

6.0 0.004479 0.004471 0.002367 0.002378

7.0 0.002769 0.002767 0.001404 0.001392

8.0 0.001709 0.001708 0.000804 0.000808

9.0 0.001077 0.001078 0.000492 0.000494

10.0 0.000705 0.000705 0.000323 0.000325

R (a.u.),  = 50° Y† Y Z†Z

3.0 0.029934  0.054015 

3.4  0.007654  0.006861

3.5  0.003044  0.001870

3.6  0.000211  0.008443

3.7  0.002703  0.012296

3.8  0.004786  0.014592

3.9  0.006271  0.015491

4.0 0.007244 0.007335 0.015327 0.015235

4.2  0.008045  0.013167

4.5  0.008016  0.008505

5.0 0.006752 0.006646 0.002971 0.002873

6.0 0.004340 0.004331 0.000292 0.000287

7.0 0.002685 0.002684 0.000471 0.000475

8.0 0.001657 0.001658 0.000318 0.000322

9.0 0.001048 0.001049 0.000206 0.000207

10.0 0.000687 0.000687 0.000140 0.000141

R (a.u.),  = 55° Y† Y Z†Z

3.0 0.041257  0.044702 

3.4  0.013169  0.008448

3.5  0.007982  0.017070

3.6  0.004063  0.022079

3.7  0.000425  0.024566

3.8  0.002000  0.026670

3.9  0.003422  0.026582

4.0 0.005128 0.005063 0.025407 0.025466

4.2  0.006568  0.022215

4.5  0.006950  0.015155

5.0 0.006221 0.006221 0.007382 0.007443

6.0 0.004078 0.004071 0.001559 0.001568

7.0 0.002525 0.002523 0.000379 0.000377

8.0 0.001559 0.001560 0.000133 0.000129

9.0 0.000988 0.000989 0.000062 0.000061

10.0 0.000649 0.000792 0.000033 0.000031

R (a.u.),  = 60° Y† Y Z†Z

3.0 0.052406  0.027126 

3.4    

3.5  0.011841  0.035266

3.6  0.006930  0.038610

3.7  0.003252  0.040317

3.8  0.000181  0.039703

3.9  0.001956  0.038087

4.0 0.003478 0.003244 0.035657 0.035859

4.2  0.004555  0.029995

4.5  0.006065  0.021192

5.0 0.005574 0.005538 0.011220 0.011189

6.0 0.003707 0.003725 0.003163 0.003160

7.0 0.002296 0.002294 0.001129 0.001128

8.0 0.001418 0.001420 0.000538 0.000534

9.0 0.000901 0.000901 0.000306 0.000305

10.0 0.000593 0.000592 0.000191 0.000189

R (a.u.),  = 65° Y† Y Z†Z

3.0 0.063615  0.000980 

3.4  0.020140  0.052356

3.5  0.013538  0.055779

3.6  0.008250  0.056594

3.7  0.004246  0.055270

3.8  0.001393  0.052774

3.9  0.000730  0.049114

4.0 0.002287 0.002286 0.045150 0.044918

4.2  0.004129  0.036708

4.5  0.005071  0.026492

5.0 0.004824 0.004822 0.014434 0.014373

6.0 0.003238 0.003233 0.004509 0.004530

7.0 0.002007 0.002005 0.001771 0.001771

8.0 0.001240 0.001242 0.000889 0.000885

9.0 0.000789 0.000790 0.000520 0.000519

10.0 0.000520 0.000563 0.000331 0.000329

R (a.u.),  = 70° Y† Y Z†Z

3.0 0.065844  0.037993 

3.4  0.019707  0.076350

3.5  0.013310  0.075604

3.6  0.008309  0.073003

3.7  0.004671  0.068750

3.8  0.001942  0.063834

3.9  0.000045  0.058575

4.0 0.001473 0.001499 0.053269 0.053024

4.2  0.003172  0.043295

4.5  0.004095  0.030832

5.0 0.003981 0.003979 0.017015 0.016985

6.0 0.002689 0.002685 0.005595 0.005634

7.0 0.001667 0.001667 0.002299 0.002299

8.0 0.001030 0.001032 0.001181 0.001178

9.0 0.000656 0.000657 0.000700 0.000698

10.0 0.000433 0.000477 0.000449 0.000449

R (a.u.),  = 75° Y† Y Z†Z

3.0 0.063550  0.085075 

3.4  0.017062  0.097846

3.5  0.011407  0.092830

3.6  0.007213  0.086637

3.7  0.004128  0.080017

3.8  0.001900  0.073102

3.9  0.000247  0.066349

4.0 0.000923 0.000885 0.059688 0.059841

4.2  0.002150  0.047829

4.5  0.003104  0.034080

5.0 0.003059 0.003116 0.018980 0.018804

6.0 0.002074 0.002071 0.006429 0.006478

7.0 0.001286 0.001288 0.002709 0.002705

8.0 0.000795 0.000796 0.001411 0.001408

9.0 0.000507 0.000508 0.000842 0.000840

10.0 0.000335 0.000335 0.000544 0.000543

R (a.u.),  = 80° Y† Y Z†Z

3.0 0.051275  0.131702 

3.4  0.012419  0.114393

3.5  0.008252  0.105760

3.6  0.005157  0.096809

3.7  0.003027  0.088010

3.8  0.001430  0.079573

3.9  0.000284  0.071645

4.0 0.000541 0.000539 0.064278 0.064299

4.2  0.001528  0.051346

4.5  0.002086  0.036404

5.0 0.002075 0.002072 0.020356 0.020515

6.0 0.001410 0.001430 0.007016 0.007036

7.0 0.000874 0.000876 0.003002 0.002998

8.0 0.000541 0.000542 0.001577 0.001574

9.0 0.000345 0.000345 0.000946 0.000942

10.0 0.000228 0.000204 0.000613 0.000610

R (a.u.),  = 85° Y† Y Z†Z

3.0 0.028985  0.167934 

3.4  0.006477  0.124900

3.5  0.004313  0.113697

3.6  0.002732  0.103013

3.7  0.001590  0.092931

3.8  0.000766  0.083558

3.9  0.000173  0.074906

4.0 0.000251 0.000251 0.067014 0.067087

4.2  0.000759  0.053390

4.5  0.001051  0.037730

5.0 0.001049 0.001011 0.021168 0.021181

6.0 0.000713 0.000713 0.007365 0.007365

7.0 0.000442 0.000443 0.003178 0.003174

8.0 0.000274 0.000274 0.001676 0.001675

9.0 0.000175 0.000175 0.001008 0.001006

10.0 0.000116 0.000072 0.000655 0.000653

R (a.u.),  = 90° Y† Y Z†Z

3.0 0  0.181782 

3.4  0  0.128472

3.5  0  0.116398

3.6  0  0.104900

3.7  0  0.094549

3.8  0  0.084856

3.9  0  0.075987

4.0 0 0 0.067927 0.067919

4.2  0  0.054041

4.5  0  0.038162

5.0 0 0 0.021437 0.021335

6.0 0 0 0.007481 0.007472

7.0 0 0 0.003236 0.003233

8.0 0 0 0.001710 0.001707

9.0 0 0 0.001029 0.001027

10.0 0 0 0.000669 0.000666

**Table S10.** Comparison of Cartesian components of the dipole moment of H2 ⋅ ⋅ ⋅ H in this work with the results of Gustafsson, Frommhold, and Meyer (GFM). We have reoriented the H2-H complex in our work to correspond to the orientation used by GFM. † designates our calculations with the aug-cc-pV5Z basis set, with Molpro 2012 and the tighter convergence criteria. We obtained values marked \* with the default convergence criteria. The H-H bond length is r = 1.111 a.u., the angle between the H2 bond axis and the pair-fixed Z axis is  (see text), and the distance between the H2 center of mass and the H nucleus is R.

R (a.u.),  = 0° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.101942 0.102416

3.5 0 0 0.052309\* 0.052670

4.0 0 0 0.023702 0.023933

4.5 0 0 0.009230\* 0.009368

5.0 0 0 0.002443 0.002527

6.0 0 0 0.001493 0.001452

7.0 0 0 0.001552 0.001533

8.0 0 0 0.001067 0.001062

9.0 0 0 0.000688 0.000685

10.0 0 0 0.000451 0.000446

R (a.u.),  = 30° X† X (GFM)Z†Z (GFM)

3.0 0.010413 0.009870 0.115388 0.115030

3.5 0.006979\* 0.006544 0.061114\* 0.059924

4.0 0.004868 0.004550 0.029651 0.027883

4.5 0.003483\* 0.003268 0.013245\* 0.011899

5.0 0.002525 0.002296 0.005170 0.004707

6.0 0.001360 0.001128 0.000171 0.000136

7.0 0.000762 0.000678 0.000851 0.000794

8.0 0.000450 0.000413 0.000665 0.000632

9.0 0.000281 0.000262 0.000441 0.000419

10.0 0.000184 0.000173 0.000289 0.000274

R (a.u.),  =60° X† X (GFM)Z†Z (GFM)

3.0 0.009761 0.009266 0.142451 0.141746

3.5 0.006625\* 0.006286 0.078045\* 0.076804

4.0 0.004668 0.004526 0.040877 0.039176

4.5 0.003362\* 0.003167 0.020793\* 0.019442

5.0 0.002448 0.002027 0.010310 0.009847

6.0 0.001328 0.001034 0.002358 0.002335

7.0 0.000748 0.000655 0.000506 0.000528

8.0 0.000444 0.000405 0.000121 0.000136

9.0 0.000276 0.000258 0.000048 0.000054

10.0 0.000181 0.000171 0.000030 0.000035

R (a.u.),  =90° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.155900 0.156280

3.5 0 0 0.086123\* 0.086408

4.0 0 0 0.046150 0.046338

4.5 0 0 0.024333 0.024459

5.0 0 0 0.012729 0.012811

6.0 0 0 0.003562 0.003594

7.0 0 0 0.001164 0.001173

8.0 0 0 0.000506 0.000510

9.0 0 0 0.000289 0.000290

10.0 0 0 0.000190 0.000189

**Table S11.** Comparison of Cartesian components of the dipole moment of H2 ⋅ ⋅ ⋅ H in this work with the results of Gustafsson, Frommhold, and Meyer (GFM). We have reoriented the H2-H complex in our work to correspond to the orientation used by GFM. † designates our calculations with the aug-cc-pV5Z basis set, with Molpro 2012 and the tighter convergence criteria. We obtained values marked \* with the default convergence criteria. The H-H bond length is r = 1.280 a.u., the angle between the H2 bond axis and the pair-fixed Z axis is  (see text), and the distance between the H2 center of mass and the H nucleus is R.

R (a.u.),  = 0° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.087531 0.088058

3.5 0 0 0.044625\* 0.045068

4.0 0 0 0.018453 0.018742

4.5 0 0 0.005628 0.005798

5.0 0 0 0.000036 0.000135

6.0 0 0 0.002573 0.002527

7.0 0 0 0.002089 0.002068

8.0 0 0 0.001367 0.001362

9.0 0 0 0.000871 0.000868

10.0 0 0 0.000569 0.000564

R (a.u.),  = 30° X† X (GFM)Z†Z (GFM)

3.0 0.012798 0.012027 0.105896 0.105856

3.5 0.008664\* 0.008029 0.056787\* 0.055629

4.0 0.006045 0.005572 0.026735 0.024764

4.5 0.004342\* 0.004062 0.011198\* 0.009400

5.0 0.003166 0.002892 0.003778 0.002973

6.0 0.001724 0.001437 0.000806 0.000850

7.0 0.000973 0.000869 0.001172 0.001129

8.0 0.000576 0.000531 0.000846 0.000815

9.0 0.000360 0.000336 0.000552 0.000531

10.0 0.000236 0.000222 0.000362 0.000346

R (a.u.),  = 60° X† X (GFM)Z†Z (GFM)

3.0 0.011564 0.010875 0.144083 0.143298

3.5 0.008022\* 0.007517 0.080176\* 0.078762

4.0 0.005711 0.005464 0.042117 0.040144

4.5 0.004150\* 0.005464 0.021445\* 0.019582

5.0 0.003047 0.002552 0.010676 0.009860

6.0 0.001673 0.001311 0.002510 0.002410

7.0 0.000948 0.000834 0.000583 0.000585

8.0 0.000563 0.000517 0.000164 0.000172

9.0 0.000351 0.000330 0.000074 0.000076

10.0 0.000230 0.000219 0.000046 0.000048

R (a.u.),  = 90° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.163388 0.163780

3.5 0 0 0.091265\* 0.091566

4.0 0 0 0.049210 0.049406

4.5 0 0 0.026149\* 0.026272

5.0 0 0 0.013851 0.013929

6.0 0 0 0.004064 0.004092

7.0 0 0 0.001422 0.001429

8.0 0 0 0.000652 0.000656

9.0 0 0 0.000379 0.000379

10.0 0 0 0.000248 0.000247

**Table S12.** Comparison of Cartesian components of the dipole moment of H2 ⋅ ⋅ ⋅ H in this work with the results of Gustafsson, Frommhold, and Meyer (GFM). We have reoriented the H2-H complex in our work to correspond to the orientation used by GFM. † designates our calculations with the aug-cc-pV5Z basis set, with Molpro 2012 and the tighter convergence criteria. We obtained values marked \* with the default convergence criteria. The H-H bond length is r = 1.449 a.u., the angle between the H2 bond axis and the pair-fixed Z axis is  (see text), and the distance between the H2 center of mass and the H nucleus is R.

R (a.u.),  = 0° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.068855 0.069411

3.5 0 0 0.034992\* 0.035530

4.0 0 0 0.011906 0.012267

4.5 0 0 0.001161\* 0.001367

5.0 0 0 0.002905 0.002792

6.0 0 0 0.003829 0.003781

7.0 0 0 0.002683 0.002662

8.0 0 0 0.001689 0.001684

9.0 0 0 0.001064 0.001061

10.0 0 0 0.000693 0.000688

R (a.u.),  = 30° X† X (GFM)Z†Z (GFM)

3.0 0.014908 0.013912 0.092080 0.092580

3.5 0.010327\* 0.009463 0.050876\* 0.049865

4.0 0.007211 0.006546 0.022959 0.020867

4.5 0.005195\* 0.004811 0.008620\* 0.006361

5.0 0.003811 0.003491 0.002064 0.000860

6.0 0.002101 0.001746 0.001544 0.001708

7.0 0.001194 0.001065 0.001524 0.001506

8.0 0.000708 0.000654 0.001038 0.001013

9.0 0.000442 0.000414 0.000669 0.000649

10.0 0.000290 0.000274 0.000438 0.000421

R (a.u.),  = 60° X† X (GFM)Z†Z (GFM)

3.0 0.012731 0.011852 0.143668 0.142866

3.5 0.009222\* 0.008541 0.081857\* 0.080270

4.0 0.006677 0.006297 0.043229 0.040993

4.5 0.004907 0.004666 0.022026 0.019664

5.0 0.003638 0.003073 0.011002 0.009779

6.0 0.002025 0.001575 0.002654 0.002450

7.0 0.001156 0.001016 0.000662 0.000638

8.0 0.000689 0.000633 0.000210 0.000210

9.0 0.000430 0.000405 0.000101 0.000100

10.0 0.000282 0.000269 0.000063 0.000065

R (a.u.),  = 90° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.170623 0.171036

3.5 0 0 0.096544\* 0.096864

4.0 0 0 0.052405 0.052610

4.5 0 0 0.028028 0.028156

5.0 0 0 0.015011 0.015089

6.0 0 0 0.004580 0.004606

7.0 0 0 0.001690 0.001696

8.0 0 0 0.000805 0.000808

9.0 0 0 0.000473 0.000472

10.0 0 0 0.000308 0.000308

**Table S13.** Comparison of Cartesian components of the dipole moment of H2 ⋅ ⋅ ⋅ H in this work with the results of Gustafsson, Frommhold, and Meyer (GFM). We have reoriented the H2-H complex in our work to correspond to the orientation used by GFM. † designates our calculations with the aug-cc-pV5Z basis set, with Molpro 2012 and the tighter convergence criteria. We obtained values marked \* with the default convergence criteria. The H-H bond length is r = 1.618 a.u., the angle between the H2 bond axis and the pair-fixed Z axis is  (see text), and the distance between the H2 center of mass and the H nucleus is R.

R (a.u.),  = 0° X† X (GFM)Z†Z (GFM)

3.0 0  0.046922 0.047510

3.5    0.024524

4.0 0  0.004188 0.004629

4.5    0.003933

5.0 0  0.006399 0.006275

6.0 0  0.005262 0.005215

7.0 0  0.003327 0.003308

8.0 0  0.002027 0.002023

9.0 0  0.001262 0.001262

10.0 0  0.000820 0.000816

R (a.u.),  = 30° X† X (GFM)Z†Z (GFM)

3.0 0.016445 0.015258 0.073606 0.074907

3.5  0.010808  0.042672

4.0 0.008333 0.007448 0.018333 0.016260

4.5  0.005485  0.002842

5.0 0.004437 0.004073 0.000028 0.001610

6.0 0.002480 0.002045 0.002381 0.002724

7.0 0.001420 0.001258 0.001900 0.001921

8.0 0.000844 0.000778 0.001236 0.001221

9.0 0.000527 0.000494 0.000787 0.000770

10.0 0.000345 0.000326 0.000514 0.000498

R (a.u.),  =60° X† X (GFM)Z†Z (GFM)

3.0 0.012798 0.011776 0.140356 0.139652

3.5  0.009230  0.081119

4.0 0.007501 0.006984 0.044153 0.041674

4.5  0.005317  0.019710

5.0 0.004195 0.003582 0.011283 0.009613

6.0 0.002372 0.001812 0.002786 0.002449

7.0 0.001366 0.001192 0.000741 0.000684

8.0 0.000816 0.000748 0.000258 0.000248

9.0 0.000511 0.000480 0.000130 0.000126

10.0 0.000335 0.000320 0.000081 0.000082

R (a.u.),  =90° X† X (GFM)Z†Z (GFM)

3.0 0  0.177316 0.177746

3.5    0.102133

4.0 0  0.055659 0.055881

4.5    0.030090

5.0 0  0.016187 0.016267

6.0 0  0.005100 0.005126

7.0 0  0.001961 0.001969

8.0 0  0.000961 0.000965

9.0 0  0.000569 0.000568

10.0 0  0.000370 0.000369

**Table S14.** Comparison of Cartesian components of the dipole moment of H2 ⋅ ⋅ ⋅ H in this work with the results of Gustafsson, Frommhold, and Meyer (GFM). We have reoriented the H2-H complex in our work to correspond to the orientation used by GFM. † designates our calculations with the aug-cc-pV5Z basis set, with Molpro 2012 and the tighter convergence criteria. We obtained values marked \* with the default convergence criteria. The H-H bond length is r = 1.787 a.u., the angle between the H2 bond axis and the pair-fixed Z axis is  (see text), and the distance between the H2 center of mass and the H nucleus is R.

R (a.u.),  = 0° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.024249 0.024865

3.5 0 0 0.012493\* 0.013214

4.0 0 0 0.004298 0.003764

4.5 0 0 0.010297 0.010009

5.0 0 0 0.010436 0.010301

6.0 0 0 0.006866 0.006828

7.0 0 0 0.004014 0.004001

8.0 0 0 0.002373 0.002375

9.0 0 0 0.001461 0.001468

10.0 0 0 0.000946 0.000947

R (a.u.),  = 30° X† X (GFM)Z†Z (GFM)

3.0 0.017027 0.015733 0.050826 0.053158

3.5 0.013393\* 0.012036 0.034367\* 0.034277

4.0 0.009398 0.008272 0.012957 0.011106

4.5 0.006772\* 0.006066 0.001891\* 0.001042

5.0 0.005020 0.004620 0.002317 0.004381

6.0 0.002845 0.002328 0.003307 0.003906

7.0 0.001644 0.001439 0.002296 0.002371

8.0 0.000980 0.000899 0.001436 0.001436

9.0 0.000612 0.000571 0.000903 0.000894

10.0 0.000400 0.000377 0.000589 0.000577

R (a.u.),  = 60° X† X (GFM)Z†Z (GFM)

3.0 0.011162 0.010875 0.133086 0.143298

3.5 0.010411\* 0.009436 0.082868\* 0.081041

4.0 0.008116 0.007479 0.044810 0.042126

4.5 0.006180\* 0.005839 0.022954\* 0.019731

5.0 0.004695 0.004064 0.011514 0.009378

6.0 0.002702 0.002009 0.002905 0.002398

7.0 0.001571 0.001351 0.000819 0.000716

8.0 0.000942 0.000853 0.000307 0.000279

9.0 0.000591 0.000549 0.000160 0.000149

10.0 0.000388 0.000365 0.000100 0.000096

R (a.u.),  = 90° X† X (GFM)Z†Z (GFM)

3.0 0 0 0.183115 0.183584

3.5 0 0 0.106778\* 0.107151

4.0 0 0 0.058862 0.059102

4.5 0 0 0.031867\* 0.032012

5.0 0 0 0.017350 0.017434

6.0 0 0 0.005610 0.005636

7.0 0 0 0.002228 0.002237

8.0 0 0 0.001116 0.001120

9.0 0 0 0.000663 0.000664

10.0 0 0 0.000431 0.000431

Table S15. Comparison of results obtained with the aug-cc-pV5Z (A5Z), aug-cc-pV6Z (A6Z), and d-aug-cc-pV5Z (D5Z) basis sets for the components of the dipole of H2 ⋅ ⋅ ⋅ H in the y and z directions, with an H-H bond length of 1.449 a.u. The center of mass of H2 and the H nucleus are separated by the distance R along the z axis, and the angle between the bond axis of H2 and the z axis is . All results have been obtained at RHF/UCCSD(T) level.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |
| R = 3.0 a.u. |  | | |  | | |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 |  | 0.068855 | 0.068855 |  |
| 5° | 0.003223 | 0.003223 |  | 0.069519 | 0.069517 |  |
| 10° | 0.006305 | 0.006304 |  | 0.071520 | 0.071528 |  |
| 15° | 0.009114 | 0.009109 |  | 0.074838 | 0.074846 |  |
| 20° | 0.011538 | 0.011527 |  | 0.079425 | 0.079441 |  |
| 25° | 0.013487 | 0.013474 | 0.013481 | 0.085214 | 0.085225 | 0.085233 |
| 30° | 0.014908 | 0.014894 | 0.014917 | 0.092080 | 0.092087 | 0.092112 |
| 35° | 0.015777 | 0.015764 | 0.015766 | 0.099876 | 0.099869 | 0.099856 |
| 40° | 0.016100 | 0.016088 | 0.016100 | 0.108343 | 0.108352 | 0.108382 |
| 45° | 0.015905 | 0.015895 | 0.015901 | 0.117267 | 0.117267 | 0.117271 |
| 50° | 0.015239 | 0.015231 | 0.015261 | 0.126328 | 0.126330 | 0.126340 |
| 55° | 0.014161 | 0.014153 | 0.014151 | 0.135236 | 0.135232 | 0.135234 |
| 60° | 0.012731 | 0.012724 | 0.012720 | 0.143668 | 0.143664 | 0.143671 |
| 65° | 0.011012 | 0.011007 | 0.011004 | 0.151335 | 0.151331 | 0.151343 |
| 70° | 0.009065 | 0.009060 | 0.009063 | 0.157986 | 0.157981 | 0.157977 |
| 75° | 0.006942 | 0.006939 | 0.006939 | 0.163386 | 0.163382 | 0.163383 |
| 80° | 0.004695 | 0.004693 | 0.004694 | 0.167361 | 0.167370 | 0.167376 |
| 85° | 0.002367 | 0.002366 | 0.002370 | 0.169807 | 0.169804 | 0.169809 |
| 90° | 0 | 0 | 0.000001 | 0.170623 | 0.170628 | 0.170632 |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |
| R = 4.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0.000025 | 0.011906 | 0.011906 |  |
| 5° | 0.001509 | 0.001500 |  | 0.012250 | 0.012255 |  |
| 10° | 0.002957 | 0.002943 | 0.002948 | 0.013269 | 0.013275 | 0.013268 |
| 15° | 0.004294 | 0.004277 | 0.004274 | 0.014923 | 0.014930 | 0.014942 |
| 20° | 0.005472 | 0.005455 | 0.005466 | 0.017149 | 0.017156 | 0.017162 |
| 25° | 0.006454 | 0.006436 | 0.006444 | 0.019862 | 0.019868 | 0.019870 |
| 30° | 0.007211 | 0.007194 | 0.007208 | 0.022959 | 0.022965 | 0.022980 |
| 35° | 0.007725 | 0.007710 | 0.007717 | 0.026329 | 0.026334 | 0.026334 |
| 40° | 0.007988 | 0.007975 | 0.007979 | 0.029852 | 0.029856 | 0.029866 |
| 45° | 0.008003 | 0.007992 | 0.007998 | 0.033411 | 0.033415 | 0.033418 |
| 50° | 0.007778 | 0.007768 | 0.007774 | 0.036893 | 0.036898 | 0.036900 |
| 55° | 0.007329 | 0.007320 | 0.007327 | 0.040196 | 0.040201 | 0.040208 |
| 60° | 0.006677 | 0.006669 | 0.006678 | 0.043229 | 0.043235 | 0.043237 |
| 65° | 0.005846 | 0.005839 | 0.005846 | 0.045915 | 0.045921 | 0.045925 |
| 70° | 0.004862 | 0.004856 | 0.004861 | 0.048191 | 0.048198 | 0.048199 |
| 75° | 0.003755 | 0.003751 | 0.003753 | 0.050009 | 0.050016 | 0.050016 |
| 80° | 0.002556 | 0.002553 | 0.002556 | 0.051332 | 0.051339 | 0.051339 |
| 85° | 0.001293 | 0.001292 | 0.001295 | 0.052136 | 0.052142 | 0.052142 |
| 90° | 0 | 0 | 0 | 0.052405 | 0.052411 | 0.052410 |
|  |  |  |  |  |  |  |

Table S15. (*Continued.)*

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|  |  |  |  |  |  |  |
| R = 5.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0.000003 | 0.002905 | 0.002905 | 0.002897 |
| 5° | 0.000786 | 0.000782 | 0.000807 | 0.002749 | 0.002745 | 0.002724 |
| 10° | 0.001542 | 0.001536 | 0.001538 | 0.002288 | 0.002284 | 0.002279 |
| 15° | 0.002243 | 0.002237 | 0.002239 | 0.001540 | 0.001536 | 0.001532 |
| 20° | 0.002868 | 0.002861 | 0.002863 | 0.000537 | 0.000534 | 0.000531 |
| 25° | 0.003395 | 0.003389 | 0.003392 | 0.000680 | 0.000683 | 0.000685 |
| 30° | 0.003811 | 0.003806 | 0.003808 | 0.002064 | 0.002066 | 0.002068 |
| 35° | 0.004104 | 0.004099 | 0.004101 | 0.003563 | 0.003564 | 0.003565 |
| 40° | 0.004267 | 0.004261 | 0.004262 | 0.005123 | 0.005124 | 0.005126 |
| 45° | 0.004298 | 0.004292 | 0.004293 | 0.006694 | 0.006695 | 0.006696 |
| 50° | 0.004199 | 0.004193 | 0.004194 | 0.008225 | 0.008227 | 0.008228 |
| 55° | 0.003976 | 0.003969 | 0.003971 | 0.009674 | 0.009676 | 0.009675 |
| 60° | 0.003638 | 0.003632 | 0.003633 | 0.011002 | 0.011004 | 0.011002 |
| 65° | 0.003197 | 0.003191 | 0.003195 | 0.012176 | 0.012179 | 0.012176 |
| 70° | 0.002667 | 0.002662 | 0.002666 | 0.013171 | 0.013174 | 0.013169 |
| 75° | 0.002065 | 0.002061 | 0.002065 | 0.013964 | 0.013968 | 0.013961 |
| 80° | 0.001408 | 0.001405 | 0.001407 | 0.014542 | 0.014545 | 0.014537 |
| 85° | 0.000713 | 0.000712 | 0.000714 | 0.014893 | 0.014896 | 0.014888 |
| 90° | 0 | 0 | 0 | 0.015011 | 0.015013 | 0.015006 |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |
| R = 6.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0 | 0.003829 | 0.003829 | 0.003823 |
| 5° | 0.000432 | 0.000429 | 0.000431 | 0.003758 | 0.003758 | 0.003758 |
| 10° | 0.000848 | 0.000844 | 0.000845 | 0.003547 | 0.003547 | 0.003545 |
| 15° | 0.001234 | 0.001230 | 0.001231 | 0.003205 | 0.003205 | 0.003206 |
| 20° | 0.001578 | 0.001574 | 0.001575 | 0.002744 | 0.002744 | 0.002747 |
| 25° | 0.001870 | 0.001867 | 0.001869 | 0.002184 | 0.002184 | 0.002188 |
| 30° | 0.002101 | 0.002099 | 0.002099 | 0.001544 | 0.001545 | 0.001551 |
| 35° | 0.002266 | 0.002263 | 0.002264 | 0.000849 | 0.000850 | 0.000855 |
| 40° | 0.002360 | 0.002357 | 0.002357 | 0.000121 | 0.000122 | 0.000131 |
| 45° | 0.002381 | 0.002378 | 0.002379 | 0.000614 | 0.000613 | 0.000604 |
| 50° | 0.002330 | 0.002327 | 0.002327 | 0.001336 | 0.001335 | 0.001324 |
| 55° | 0.002210 | 0.002206 | 0.002208 | 0.002022 | 0.002021 | 0.002009 |
| 60° | 0.002025 | 0.002021 | 0.002023 | 0.002654 | 0.002653 | 0.002640 |
| 65° | 0.001782 | 0.001778 | 0.001780 | 0.003215 | 0.003214 | 0.003199 |
| 70° | 0.001488 | 0.001485 | 0.001486 | 0.003693 | 0.003692 | 0.003677 |
| 75° | 0.001154 | 0.001151 | 0.001152 | 0.004075 | 0.004074 | 0.004059 |
| 80° | 0.000787 | 0.000785 | 0.000786 | 0.004354 | 0.004353 | 0.004337 |
| 85° | 0.000399 | 0.000398 | 0.000398 | 0.004523 | 0.004523 | 0.004508 |
| 90° | 0 | 0 | 0 | 0.004580 | 0.004580 | 0.004564 |
|  |  |  |  |  |  |  |

Table S15. (*Continued.)*

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|  |  |  |  |  |  |  |
| R = 7.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0 | 0.002683 | 0.002683 | 0.002694 |
| 5° | 0.000246 | 0.000243 | 0.000243 | 0.002647 | 0.002649 | 0.002657 |
| 10° | 0.000482 | 0.000478 | 0.000481 | 0.002541 | 0.002542 | 0.002552 |
| 15° | 0.000702 | 0.000697 | 0.000700 | 0.002368 | 0.002369 | 0.002381 |
| 20° | 0.000897 | 0.000893 | 0.000897 | 0.002135 | 0.002136 | 0.002150 |
| 25° | 0.001063 | 0.001059 | 0.001063 | 0.001850 | 0.001850 | 0.001866 |
| 30° | 0.001194 | 0.001192 | 0.001197 | 0.001524 | 0.001524 | 0.001541 |
| 35° | 0.001288 | 0.001286 | 0.001290 | 0.001166 | 0.001167 | 0.001187 |
| 40° | 0.001342 | 0.001341 | 0.001344 | 0.000791 | 0.000791 | 0.000809 |
| 45° | 0.001355 | 0.001354 | 0.001357 | 0.000409 | 0.000410 | 0.000428 |
| 50° | 0.001327 | 0.001326 | 0.001329 | 0.000032 | 0.000034 | 0.000052 |
| 55° | 0.001260 | 0.001259 | 0.001260 | 0.000328 | 0.000326 | 0.000307 |
| 60° | 0.001156 | 0.001155 | 0.001156 | 0.000662 | 0.000659 | 0.000640 |
| 65° | 0.001019 | 0.001018 | 0.001018 | 0.000960 | 0.000957 | 0.000938 |
| 70° | 0.000852 | 0.000851 | 0.000851 | 0.001214 | 0.001211 | 0.001193 |
| 75° | 0.000661 | 0.000660 | 0.000660 | 0.001419 | 0.001415 | 0.001398 |
| 80° | 0.000451 | 0.000450 | 0.000450 | 0.001568 | 0.001564 | 0.001546 |
| 85° | 0.000229 | 0.000233 | 0.000228 | 0.001660 | 0.001655 | 0.001638 |
| 90° | 0 | 0 | 0 | 0.001690 | 0.001686 | 0.001668 |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |
| R = 8.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0 | 0.001689 | 0.001689 | 0.001710 |
| 5° | 0.000146 | 0.000144 | 0.000090 | 0.001669 | 0.001672 | 0.001690 |
| 10° | 0.000286 | 0.000284 | 0.000285 | 0.001610 | 0.001612 | 0.001633 |
| 15° | 0.000416 | 0.000413 | 0.000415 | 0.001513 | 0.001515 | 0.001534 |
| 20° | 0.000532 | 0.000529 | 0.000532 | 0.001383 | 0.001384 | 0.001405 |
| 25° | 0.000630 | 0.000628 | 0.000632 | 0.001223 | 0.001224 | 0.001245 |
| 30° | 0.000708 | 0.000707 | 0.000711 | 0.001038 | 0.001040 | 0.001060 |
| 35° | 0.000764 | 0.000763 | 0.000767 | 0.000836 | 0.000838 | 0.000858 |
| 40° | 0.000797 | 0.000796 | 0.000800 | 0.000622 | 0.000624 | 0.000646 |
| 45° | 0.000805 | 0.000805 | 0.000807 | 0.000404 | 0.000407 | 0.000428 |
| 50° | 0.000789 | 0.000789 | 0.000792 | 0.000189 | 0.000191 | 0.000212 |
| 55° | 0.000750 | 0.000750 | 0.000752 | 0.000018 | 0.000015 | 0.000005 |
| 60° | 0.000689 | 0.000688 | 0.000690 | 0.000210 | 0.000207 | 0.000188 |
| 65° | 0.000607 | 0.000607 | 0.000608 | 0.000382 | 0.000379 | 0.000362 |
| 70° | 0.000508 | 0.000508 | 0.000508 | 0.000529 | 0.000526 | 0.000509 |
| 75° | 0.000394 | 0.000394 | 0.000394 | 0.000647 | 0.000645 | 0.000630 |
| 80° | 0.000269 | 0.000269 | 0.000269 | 0.000734 | 0.000732 | 0.000717 |
| 85° | 0.000137 | 0.000137 | 0.000136 | 0.000787 | 0.000785 | 0.000770 |
| 90° | 0 | 0 | 0 | 0.000805 | 0.000803 | 0.000789 |
|  |  |  |  |  |  |  |

Table S15. (*Continued.)*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |
| R = 9.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0 | 0.001064 | 0.001063 | 0.001081 |
| 5° | 0.000091 | 0.000090 | 0.000058 | 0.001051 | 0.001051 | 0.001069 |
| 10° | 0.000178 | 0.000177 | 0.000177 | 0.001016 | 0.001015 | 0.001033 |
| 15° | 0.000260 | 0.000257 | 0.000259 | 0.000957 | 0.000956 | 0.000974 |
| 20° | 0.000332 | 0.000330 | 0.000332 | 0.000878 | 0.000877 | 0.000895 |
| 25° | 0.000394 | 0.000391 | 0.000393 | 0.000781 | 0.000779 | 0.000799 |
| 30° | 0.000442 | 0.000440 | 0.000442 | 0.000669 | 0.000667 | 0.000686 |
| 35° | 0.000477 | 0.000476 | 0.000478 | 0.000545 | 0.000544 | 0.000562 |
| 40° | 0.000498 | 0.000497 | 0.000498 | 0.000414 | 0.000413 | 0.000431 |
| 45° | 0.000503 | 0.000502 | 0.000503 | 0.000280 | 0.000279 | 0.000297 |
| 50° | 0.000493 | 0.000493 | 0.000494 | 0.000147 | 0.000147 | 0.000160 |
| 55° | 0.000468 | 0.000469 | 0.000469 | 0.000018 | 0.000019 | 0.000033 |
| 60° | 0.000430 | 0.000430 | 0.000430 | 0.000101 | 0.000100 | 0.000085 |
| 65° | 0.000379 | 0.000380 | 0.000379 | 0.000208 | 0.000206 | 0.000193 |
| 70° | 0.000318 | 0.000318 | 0.000318 | 0.000300 | 0.000297 | 0.000285 |
| 75° | 0.000247 | 0.000247 | 0.000246 | 0.000374 | 0.000371 | 0.000360 |
| 80° | 0.000168 | 0.000169 | 0.000168 | 0.000428 | 0.000425 | 0.000414 |
| 85° | 0.000085 | 0.000086 | 0.000085 | 0.000462 | 0.000458 | 0.000447 |
| 90° | 0 | 0 | 0 | 0.000473 | 0.000469 | 0.000458 |
|  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |
| R = 10.0 a.u. |  |  |  |  |  |  |
|  | A5Z | A6Z | D5Z | A5Z | A6Z | D5Z |
| 0° | 0 | 0 | 0 | 0.006930 | 0.000693 | 0.000707 |
| 5° | 0.000059 | 0.000059 | 0.000058 | 0.000685 | 0.000682 | 0.000699 |
| 10° | 0.000117 | 0.000115 | 0.000116 | 0.000662 | 0.000659 | 0.000676 |
| 15° | 0.000170 | 0.000168 | 0.000168 | 0.000625 | 0.000621 | 0.000639 |
| 20° | 0.000217 | 0.000215 | 0.000216 | 0.000573 | 0.000570 | 0.000587 |
| 25° | 0.000258 | 0.000256 | 0.000256 | 0.000511 | 0.000507 | 0.000525 |
| 30° | 0.000290 | 0.000288 | 0.000288 | 0.000438 | 0.000435 | 0.000451 |
| 35° | 0.000313 | 0.000311 | 0.000311 | 0.000358 | 0.000355 | 0.000370 |
| 40° | 0.000326 | 0.000325 | 0.000324 | 0.000273 | 0.000270 | 0.000285 |
| 45° | 0.000330 | 0.000329 | 0.000329 | 0.000186 | 0.000183 | 0.000197 |
| 50° | 0.000323 | 0.000323 | 0.000322 | 0.000099 | 0.000097 | 0.000110 |
| 55° | 0.000307 | 0.000307 | 0.000306 | 0.000015 | 0.000014 | 0.000025 |
| 60° | 0.000282 | 0.000282 | 0.000281 | 0.000063 | 0.000064 | 0.000053 |
| 65° | 0.000249 | 0.000249 | 0.000248 | 0.000133 | 0.000134 | 0.000125 |
| 70° | 0.000209 | 0.000208 | 0.000207 | 0.000194 | 0.000194 | 0.000185 |
| 75° | 0.000162 | 0.000162 | 0.000160 | 0.000243 | 0.000242 | 0.000235 |
| 80° | 0.000111 | 0.000111 | 0.000110 | 0.000279 | 0.000278 | 0.000271 |
| 85° | 0.000056 | 0.000056 | 0.000056 | 0.000301 | 0.000299 | 0.000293 |
| 90° | 0 | 0 | 0 | 0.000308 | 0.000307 | 0.000300 |
|  |  |  |  |  |  |  |

Table S16. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 0.942 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 136369 1772 12549 66 112 5 3  1

3.4 83604 1066 8815 4 114 3 0  0

3.5 73635 952 8127 3 110 2 0 1 0

3.6 64755 851 7505 7 105 2 0 1 0

3.7 56866 760 6941 11 99 2 0 0 0

3.8 49868 678 6426 13 93 2 0 0 0

3.9 43674 604 5954 14 87 2 0 0 1

4.0 38199 535 5521 14 81 1 0 0 1

4.0† 38199 535 5521 13 81 1 1 1 0

4.2 29108 418 4757 13 70 1 1 1 0

4.5 19168 282 3820 10 54 0 1 0 0

5.0 9277 140 2681 7 34 0 0 0 0

5.0† 9278 140 2681 7 34 0 0 0 0

6.0 1885 31 1381 3 13 0 0 0 0

6.0† 1885 31 1381 3 13 0 0 0 0

7.0 265 8 761 1 5 0 0 0 0

7.0† 265 8 761 1 5 0 0 0 0

8.0 23 2 446 1 1 0 0 0 0

8.0† 15 1 446 0 2 0 0 0 0

9.0 34 1 278 0 1 0 0 0 0

9.0† 35 1 278 0 1 0 0 0 0

10.0 23 2 182 0 0 0 0 0 0

10.0† 23 2 182 0 0 0 0 0 0

Table S17. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 1.111 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 137922 3659 17806 182 178 17 9 1 0

(45) 137919 3653 17799 192 171

GFM 137628 4085 17645 437 132

3.4 85241 2150 12337 22 210 8 1 1 0

3.5 75113 1917 11350 2 205 6 0 1 0

(45) 75112 1916 11348 5 203

GFM 74327 2365 11401 394 288

3.6 66063 1713 10463 12 197 5 1 1 0

3.7 58004 1532 9661 22 188 4 1 1 0

3.8 50848 1369 8931 28 177 3 1 1 0

3.9 44510 1222 8264 32 166 3 2 1 0

4.0 38908 1089 7653 34 155 2 2 1 0

4.0† 38908 1089 7653 34 155 2 2 1 0

(45) 38908 1089 7623 33 155

GFM 37734 1500 7884 442 480

4.2 29611 858 576 34 133 1 2 1 0

4.5 19467 588 5262 29 104 1 1 0 0

(45) 19467 589 5262 29 104

GFM 18545 932 5412 366 350

5.0 9410 299 3668 19 66 1 2 0 0

5.0† 9409 300 3668 19 66 0 1 0 0

(45) 9410 300 3668 19 67

GFM 9104 609 3576 185 48

6.0 1919 70 1871 6 26 0 0 0 0

6.0† 1919 70 1871 6 26 0 0 0 0

(45) 1919 70 1872 7 26

GFM 1929 246 1725 20 33

Table S17. (*Continued.)*

R D01 D21 D23 D43 D45 D65 D67 D87 D89

7.0 274 17 1025 1 10 0 0 0 0

7.0† 274 18 1025 2 10 0 0 0 0

(45) 274 17 1025 2 10

GFM 302 68 968 6 20

8.0 21 0 594 1 3 1 2 1 1

8.0† 13 4 599 0 4 0 0 0 0

(45) 12 4 600 1 4

GFM 5 25 574 5 11

9.0 34 7 379 1 2 2 1 1 1

9.0† 34 2 373 0 2 0 0 0 0

(45) 34 2 373 1 2

GFM 25 11 360 3 6

10.0 23 2 245 1 1 0 0 0 0

10.0 † 23 2 245  1 0 0 0 0

(45) 23 2 245 1 1

GFM 17 6 236 2 3

11.0, GFM 9 2 161 1 2

Table S18. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 1.280 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 137794 6568 24048 465 200 48 28 1 1

(45) 137785 6549 24028 489 181

GFM 137557 7067 23704 701 104

3.4 86279 3753 16432 83 337 21 6 2 1

3.5 76107 3338 15089 34 336 17 3 1 1

(45) 76104 3333 15084 43 331

GFM 75261 3891 15032 454 205

3.6 66969 2981 13888 2 329 13 1 1 0

3.7 58802 2666 12805 28 317 10 1 1 0

3.8 51533 2386 11823 46 302 7 2 1 0

3.9 45084 2134 10927 58 286 5 3 1 0

4.0 39381 1906 10108 65 268 4 3 1 0

4.0† 39381 1906 10108 65 268 4 4 2 0

(45) 39381 1906 10108 63 268

GFM 38036 2424 10306 471 462

4.2 29918 1511 8667 69 232 2 4 1 0

4.5 19614 1048 6909 62 182 0 4 1 1

(45) 19616 1051 6912 61 182

GFM 18346 1479 7117 456 434

5.0 9446 545 4786 41 117 0 2 0 0

5.0† 9447 544 4787 41 116 1 2 0 0

(45) 9447 545 4787 42 117

GFM 8893 942 4719 266 97

6.0 1927 131 2415 14 46 0 1 0 0

6.0† 1927 131 2415 13 46 0 1 0 0

(45) 1927 131 2416 14 46

GFM 1881 359 2248 38 32

Table S18. (*Continued.*)

R D01 D21 D23 D43 D45 D65 D67 D87 D89

7.0 279 32 1314 3 18 1 1 0 0

7.0† 279 32 1314 3 18 1 1 0 0

(45) 279 32 1314 3 18

GFM 295 97 1248 3 24

8.0 9 8 766 1 9 1 1 0 0

8.0† 9 8 766 1 9 1 0 0 0

(45) 9 8 766 1 8

GFM 4 33 737 4 13

9.0 30 4 477 0 5 0 1 0 0

9.0† 33 3 476 1 4 1 0 0 0

(45) 33 3 476 1 4

GFM 26 14 461 3 7

10.0 20 2 312 1 3 0 0 0 0

10.0† 23 2 312 1 2 0 0 0 0

(45) 23 2 312 1 2

GFM 17 7 302 2 4

11.0, GFM 9 3 206 1 2

Table S19. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 1.449 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 135447 10736 31156 1079 59 121 80 2 3

(45) 135421 10687 31100 1144 6

GFM 135348 11260 30574 1281 217

3.4 86532 5943 21022 248 466 56 22 3 2

3.5 76474 5269 19272 138 486 44 14 3 2

(45) 76466 5254 19257 162 471

GFM 75599 5914 19070 576 100

3.6 67364 4697 17716 55 490 34 8 2 1

3.7 59173 4201 16319 8 483 25 3 2 1

3.8 51853 3764 15055 51 467 20 1 1 1

3.9 45342 3372 13905 84 449 13 3 2 1

4.0 39575 3019 12853 103 425 10 4 2 0

4.0† 39575 3019 12853 102 425 10 4 2 0

(45) 39574 3017 12852 98 424

GFM 38087 3649 12984 482 392

4.2 30000 2407 11002 120 374 4 6 1 0

4.5 19590 1686 8744 113 295 1 7 2 0

(45) 19588 1687 8746 113 296

GFM 17976 2214 9002 516 492

5.0 9378 890 6022 78 190 2 4 1 1

5.0† 9378 890 6023 78 189 2 4 1 1

(45) 9379 891 6024 79 191

GFM 8538 1384 5992 347 141

6.0 1903 219 3004 25 74 0 1 0 1

6.0† 1904 219 3004 26 74 0 2 1 1

(45) 1904 219 3004 26 74

GFM 1778 516 2813 61 32

Table S19. (*Continued.)*

R D01 D21 D23 D43 D45 D65 D67 D87 D89

7.0 279 51 1622 7 30 1 1 0 0

7.0† 279 51 1622 7 30 1 1 1 0

(45) 279 51 1622 7 30

GFM 276 137 1546 1 28

8.0 6 12 942 2 14 1 1 0 0

8.0† 6 12 942 2 14 1 1 0 0

(45) 6 12 942 2 13

GFM 2 45 909 4 17

9.0 25 5 586 1 8 0 1 0 1

9.0† 31 4 585 0 7 1 0 0 0

(45) 31 5 585 0 7

GFM 26 18 567 3 8

10.0 13 1 383 0 4 0 1 1 1

10.0† 22 2 382 1 3 0 0 0 0

(45) 22 2 382 1 4

GFM 16 8 371 2 5

11.0, GFM 8 3 253 1 3

Table S20. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 1.618 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 130357 16339 38807 2325 486 261 190 1 4

(45) 130301 16232 38681 2461 600

GFM 130506 16794 37927 2470 707

3.5, GFM 75220 8416 23365 851 20

4.0† 39449 4435 15826 127  26 2 3 1

(45) 39446 4429 15821 113 618

GFM 37867 5163 15856 485 268

4.5, GFM 17458 3151 11029 538 502

5.0† 9196 1347 7359 133 291 3 8 1 0

(45) 9197 1350 7362 135 294

GFM 8043 1936 7380 413 172

6.0† 1846 337 3626 44 113 1 3 1 1

(45) 1847 338 3627 -45 114

GFM 1613 726 3416 94 33

7.0† 272 77 1941 12 45 1 2 1 0

(45) 272 77 1942 12 46

GFM 244 191 1855 6 33

8.0† 4 18 1123 4 21 1 1 0 0

(45) 4 18 1123 4 21

GFM 2 60 1085 3 21

9.0† 28 5 695 1 10 1 0 0 0

(45) 28 5 695 0 10

GFM 25 23 675 3 11

10.0† 21 2 454 0 5 0 0 0 0

(45) 21 2 454 1 5

GFM 16 10 442 2 6

11.0, GFM 8 5 301 2 4

Table S21. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 1.787 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.0† 122107 23396 46326 4674 1831 470 372 27 9

(45) 122010 23195 46083 4897 2013

GFM 127132 23366 45431 3049 542

3.4 83932 12102 30906 1454 372 313 171 14 12

3.5 74768 10624 28302 1008 578 256 126 16 13

(45) 74716 10531 28199 1150 474

GFM 74030 11290 27647 1446 82

3.6 66205 9423 26012 655 714 207 91 15 11

3.7 58324 8418 23971 381 796 162 62 13 9

3.8 51162 7555 22131 173 837 123 39 10 6

3.9 44722 6797 20456 18 849 92 22 8 5

4.0 38976 6119 18921 94 841 67 9 7 4

4.0† 38976 6119 18920 95 841 67 9 7 4

(45) 38966 6100 18902 58 821

GFM 37370 6904 18805 518 111

4.2 29388 4946 16204 223 781 33 6 4 2

4.5 18975 3539 12854 273 647 8 13 2 1

(45) 18976 3539 12856 270 651

GFM 16811 4277 13131 515 442

5.0 8891 1927 8775 213 428 6 15 1 0

5.0† 8893 1924 8771 211 425 5 13 1 0

(45) 8896 1928 8776 214 431

GFM 7422 2591 8856 452 178

6.0 1752 489 4270 72 164 2 5 0 1

6.0† 1752 489 4270 72 165 2 5 1 1

(45) 1753 -491 4272 74 167

GFM 1374 992 4045 136 36

Table S21. (*Continued.*)

R D01 D21 D23 D43 D45 D65 D67 D87 D89

7.0 257 111 2265 20 65 0 2 0 0

7.0† 257 111 2265 20 65 0 2 0 1

(45) 257 111 2266 20 66

GFM 194 263 2165 11 40

8.0 2 24 1304 6 29 1 1 0 0

8.0† 2 24 1304 7 29 1 1 0 0

(45) 2 24 1304 6 29

GFM 12 82 1259 0 27

9.0 10 10 812 8 13 8 4 2 6

9.0† 25 6 805 2 14 1 0 0 0

(45) 25 6 805 1 14

GFM 27 32 782 2 15

10.0 18 17 533 12 30 1 10 2 7

10.0† 19 2 525 0 7 0 0 0 0

(45) 19 2 525 0 7

GFM 17 15 511 1 8

11.0, GFM 9 9 347 0 5

Table S22. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 2.125 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.4 76418 19703 38792 5641 1649 1063 688 35 9

3.5 69337 16975 35660 4320 810 971 585 4 19

3.6 62175 14878 32953 3220 178 858 483 38 39

3.7 55232 13232 30562 2327 299 718 382 49 39

3.8 48668 11890 28405 1598 648 572 291 59 33

3.9 42599 10770 26447 1011 890 459 207 50 18

4.0 37077 9773 24638 553 1048 366 136 40 27

4.0† 37079 9777 24634 559 1053 360 139 42 27

4.2 27747 8089 21339 30 1187 200 50 26 13

4.5 17581 5988 17095 407 1122 66 14 13 7

5.0 7921 3397 11671 431 797 4 30 2 0

5.0† 7926 3398 11672 429 795 3 29 3 0

6.0 1452 902 5557 160 308 9 15 1 1

6.0† 1450 902 5557 162 310 8 13 0 1

7.0 201 206 2887 46 121 1 5 0 0

7.0† 201 205 2886 46 121 1 5 0 0

8.0 0 42 1643 14 53 0 2 0 0

8.0† 1 43 1643 14 52 1 1 0 0

9.0 37 3 985 14 38 10 2 2 1

9.0† 18 8 1008 4 25 1 1 0 0

10.0 36 24 630 24 43 18 24 11 15

10.0† 13 1 656 2 12 0 0 0 0

Table S23. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 2.463 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.9 39992 12941 28519 4676 879 1524 849 47 50

4.0 34855 11886 27101 3440 224 1336 745 123 66

4.0† 34855 11884 27099 3395 180 1321 698 100 82

4.2 25833 10205 24344 1514 796 859 419 143 100

4.5 15837 8167 20323 4 1356 354 97 68 45

5.0 6587 5026 14239 649 1242 52 27 19 2

5.0† 6588 5032 14255 638 1239 42 40 16 5

6.0 1006 1426 6703 297 506 26 37 6 10

6.0† 1011 1429 6710 303 514 18 28 0 1

7.0 83 313 3384 105 212 4 0 5 6

7.0† 111 330 3405 88 196 5 10 0 1

8.0 2 30 1924 39 94 33 7 29 14

8.0† 7 66 1912 26 83 0 3 0 0

9.0 3 11 1152 0 30 17 16 17 23

9.0† 12 10 1165 8 39 0 1 0 0

10.0 7 52 749 13 10 32 25 5 37

10.0† 8 0 756 3 19 0 1 0 0

Table S24. Spherical dipole coefficients DL(r, R) for H2 ⋅ ⋅ ⋅ H with r = 2.801 a.u. Coefficients in a.u., multiplied by 106.

R D01 D21 D23 D43 D45 D65 D67 D87 D89

3.9 37067 12293 24326 11187 4828 2317 1212  221

4.0 33300 10586 23224 9254 3803 2388 1244 286 191

4.0† 33325 10543 23249 9209 3795 2300 1275 334 155

4.2 25418 8787 21701 6044 1886 2304 1265 82 138

4.5 15069 7960 20093 2187 299 1343 633 242 150

5.0 5331 6045 15625 425 1455 279 4 58 28

5.0† 5345 6046 15630 437 1446 288 49 84 40

6.0 493 1971 7550 464 753 16 36 9 8

6.0† 492 1788 7675 295 911 50 31 184 173

7.0 15 477 3745 151 292 11 19 2 1

7.0† 6 469 3736 144 284 12 17 1 1

8.0 22 91 2063 40 115 2 4 1 1

8.0† 19 93 2064 41 117 2 5 0 0

9.0 10 12 1249 13 55 0 2 0 0

9.0† 7 12 1248 13 54 0 2 0 0

10.0 5 26 827 2 30 5 4 11 11

10.0† 3 1 806 5 27 0 0 1 0

Supporting Material: Figures

**Figure S1.** The first three states of the isosceles triangular H3 system with vertex angle θ = 25˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.60 a.u. H-H distance. H-H distances shorter than 1.10 a.u. are dropped, due to difficulty in convergence within the calculation.

**Figure S2.** The first three states of the isosceles triangular H3 system with vertex angle θ = 30˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.60 a.u. when the H-H distance is shorter than 1.00 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S3.** The first three states of the isosceles triangular H3 system with vertex angle θ = 35˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.40 a.u. H-H distance. When the H-H distance is shorter than 1.00 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S4.** The first three states of the isosceles triangular H3 system with vertex angle θ = 40˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.20 a.u. H-H distance. When the H-H distance is shorter than 1.00 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S5.** The first three states of the isosceles triangular H3 system with vertex angle θ = 45˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.10 a.u. H-H distance. When the H-H distance is shorter than 1.00 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S6.** The first three states of the isosceles triangular H3 system with vertex angle θ = 50˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2B2 and 2A1 states near an H-H distance of 1.20 a.u. H-H distance. When the H-H distance is shorter than 1.00 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S7.** The first three states of the isosceles triangular H3 system with vertex angle θ = 70˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.00 a.u. When the H-H distance is shorter than 0.90 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S8.** The first three states of the isosceles triangular H3 system with vertex angle θ = 75˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.00 a.u. When the H-H distance is shorter than 0.80 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S9.** The first three states of the isosceles triangular H3 system with vertex angle θ = 80˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.00 a.u. When the H-H distance is at 0.70 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S10.** The first three states of the isosceles triangular H3 system with vertex angle θ = 85˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.00 a.u. When the H-H distance is at 0.70 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S11.** The first three states of the isosceles triangular H3 system with vertex angle θ = 90˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.00 a.u. When the H-H distance is at 0.70 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S12.** The first three states of the isosceles triangular H3 system with vertex angle θ = 95˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.10 a.u. When the H-H distance is at 0.70 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S13.** The first three states of the isosceles triangular H3 system with vertex angle θ = 100˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.10 a.u. When the H-H distance is at 0.70 a.u., the energies of the three states overlap with each other on the scale of the figure.

**Figure S14.** The first three states of the isosceles triangular H3 system with vertex angle θ = 105˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.10 a.u.

**Figure S15.** The first three states of the isosceles triangular H3 system with vertex angle θ = 110˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.10 a.u.

**Figure S16.** The first three states of the isosceles triangular H3 system with vertex angle θ = 115˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.20 a.u.

**Figure S17.** The first three states of the isosceles triangular H3 system with vertex angle θ = 120˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.20 a.u.

**Figure S18.** The first three states of the isosceles triangular H3 system with vertex angle θ = 125˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.20 a.u.

**Figure S19.** The first three states of the isosceles triangular H3 system with vertex angle θ = 130˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It appears that there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.20 a.u.

**Figure S20.** The first three states of the isosceles triangular H3 system with vertex angle θ = 135˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. It looks like there is a conical intersection between the 2A1 and 2nd 2A1 states near an H-H distance of 1.30 a.u., and the two states start to split.

**Figure S21.** The first three states of the isosceles triangular H3 system with vertex angle θ = 140˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The 2A1 and 2nd 2A1 states start to split.

**Figure S22.** The first three states of the isosceles triangular H3 system with vertex angle θ = 145˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The 2A1 and 2nd 2A1 states start to split.

**Figure S23.** The first three states of the isosceles triangular H3 system with vertex angle θ = 150˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The 2A1 and 2nd 2A1 states start to split.

**Figure S24.** The first three states of the isosceles triangular H3 system with vertex angle θ = 155˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The 2A1 and 2nd 2A1 states start to split.

**Figure S25.** The first three states of the isosceles triangular H3 system with vertex angle θ = 160˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The 2A1 and 2nd 2A1 states start to split.

**Figure S26.** The first three states of the isosceles triangular H3 system with vertex angle θ = 165˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The separation of 2A1 and 2nd 2A1 states are much clearer than the previous vertex angles.

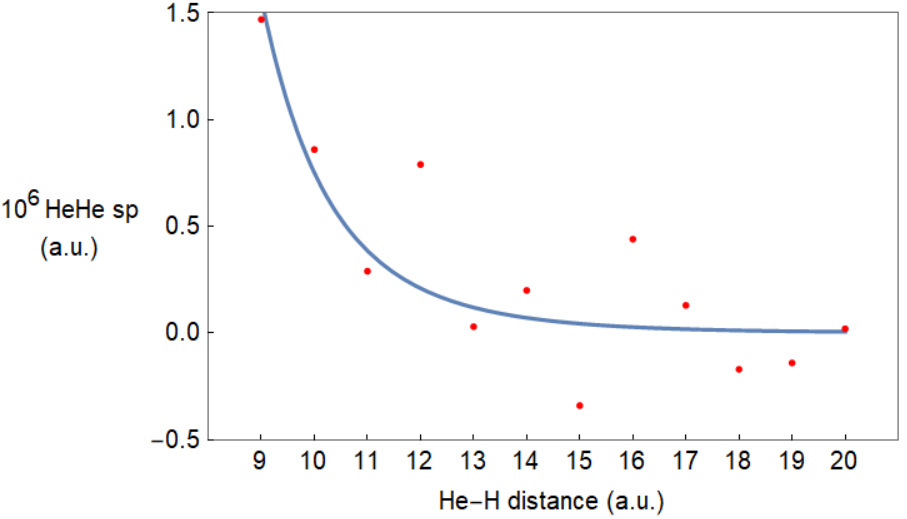
**Figure S27.** The first three states of the isosceles triangular H3 system with vertex angle θ = 170˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The separation of 2A1 and 2nd 2A1 states are visible.

**Figure S28.** The first three states of the isosceles triangular H3 system with vertex angle θ = 175˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The separation of 2A1 and 2nd 2A1 states are visible.

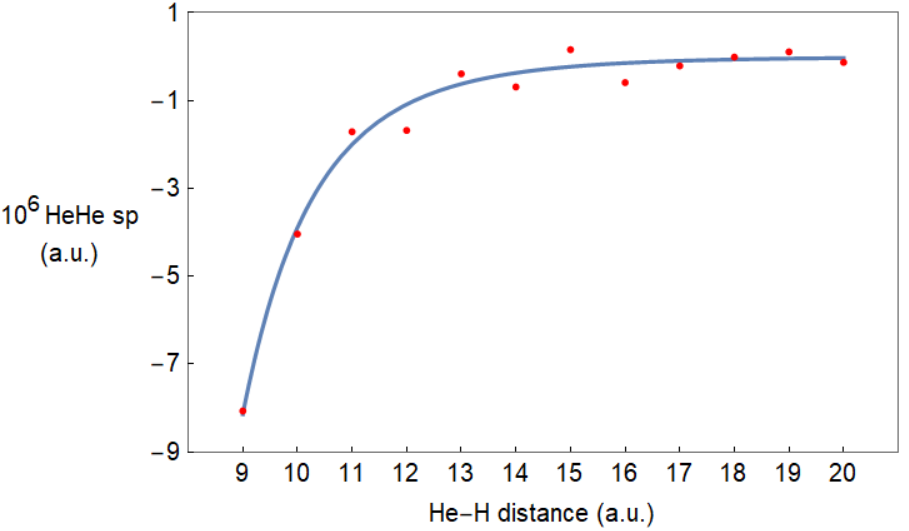
**Figure S29.** The first three states of the isosceles triangular H3 system with vertex angle θ = 180˚ at various H-H distances. The basis set for the calculation is aug-cc-pVTZ. The separation of 2A1 and 2nd 2A1 states are very distinct.

**Figure S30.** The energy of the equilateral H3 system versus the H-H distance, as obtained with the HF-FCI method.

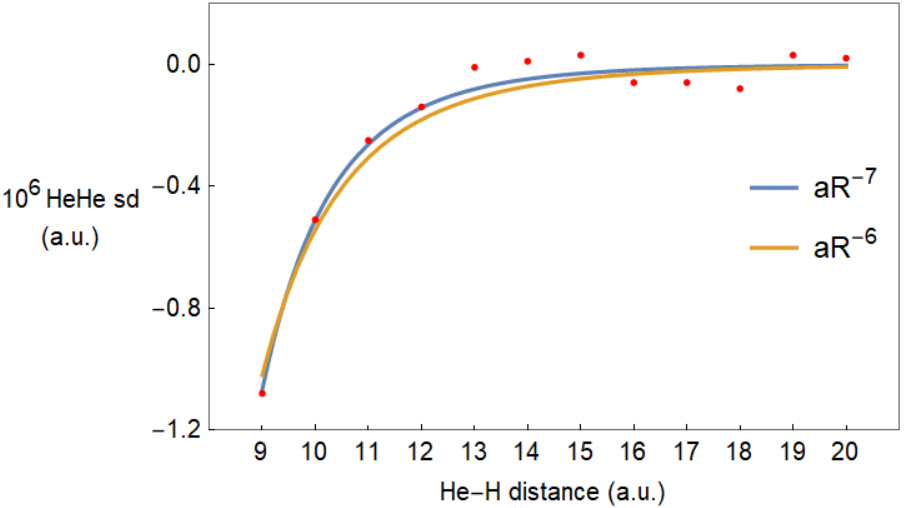
**Figure S31.** The energy of S0 and S1 for the equilateral H3 system using the method of CASSCF-FCI. The calculation started with aug-cc-pVTZ as basis set, and the results are fed into the same method but with aug-cc-pV5Z. Due to the difficulty of converging to the correct energy state, the results that are shorter than 0.89 a.u. are omitted. Literature data obtained from Ref. 78.



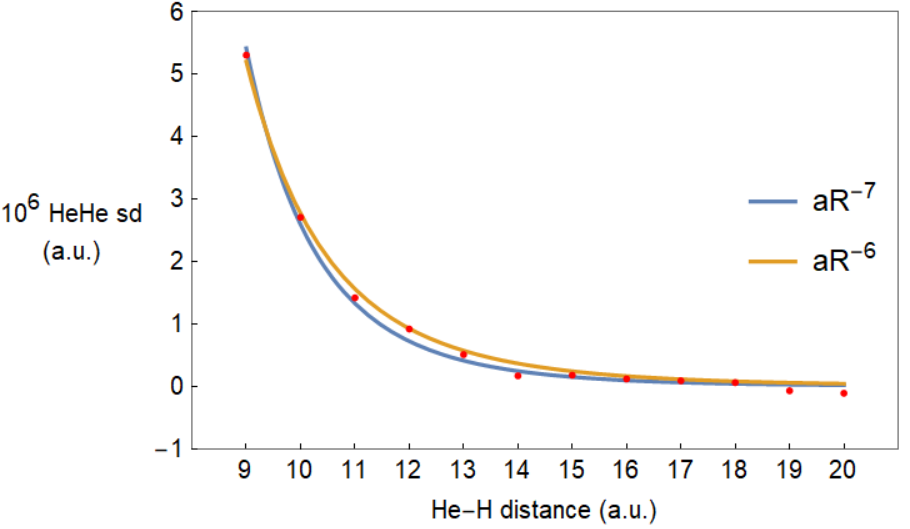
**Figure S32.** First HeHe sp correlation charge density matrix element in the list fitted with R-7, with a.u. This plot is scaled by 106.



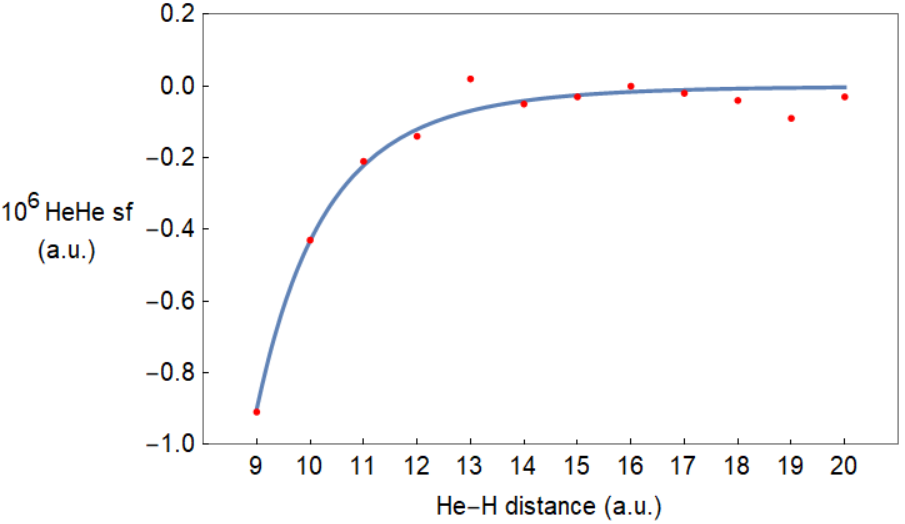
**Figure S33.** Second HeHe sp correlation charge density matrix element in the list fitted with R-7, with a.u. This plot is scaled by 106.



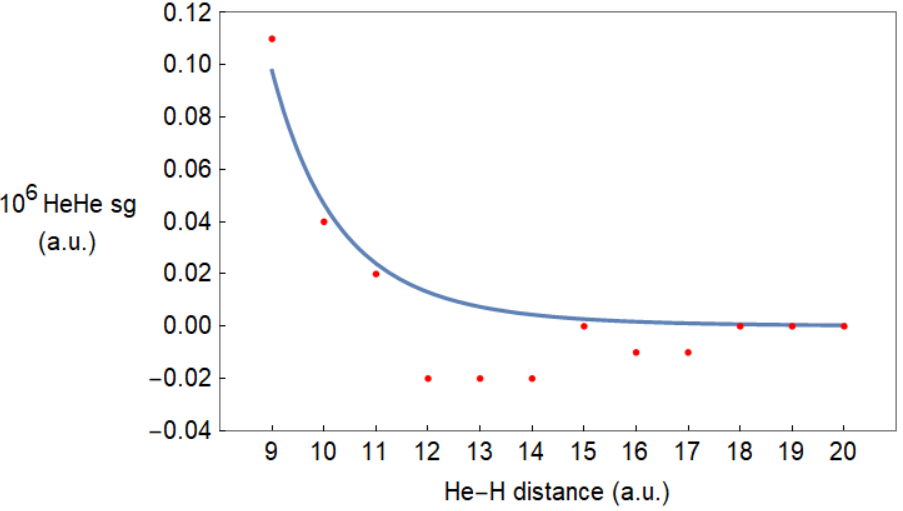
**Figure S34.** First HeHe sd correlation charge density matrix element in the list fitted with R-7 and R-6, with a.u and a.u., respectively. This plot is scaled by 106.



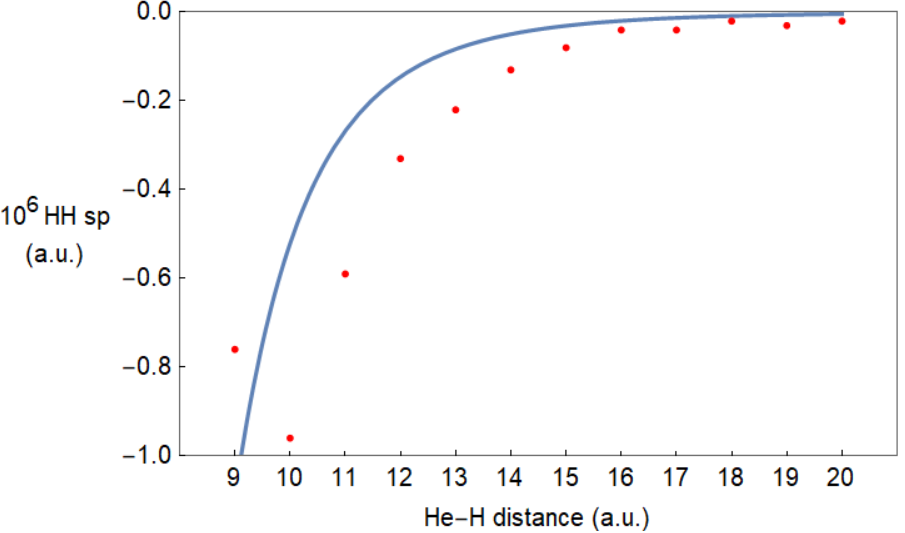
**Figure S35.** Second HeHe sd correlation charge density matrix element in the list fitted with R-7 and R-6, with a.u and a.u., respectively. This plot is scaled by 106.



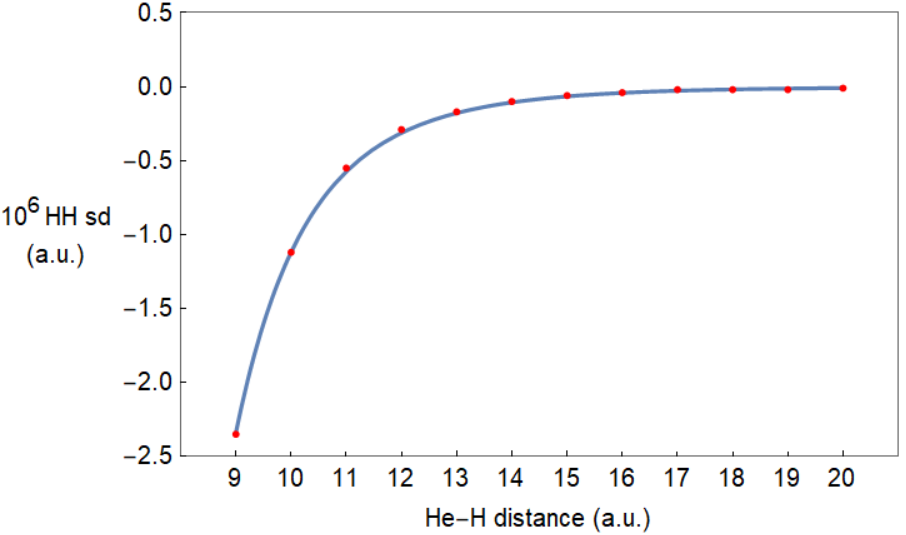
**Figure S36.** HeHe sf correlation charge density matrix elements fitted with R-7 with a.u. This plot is scaled by 106.



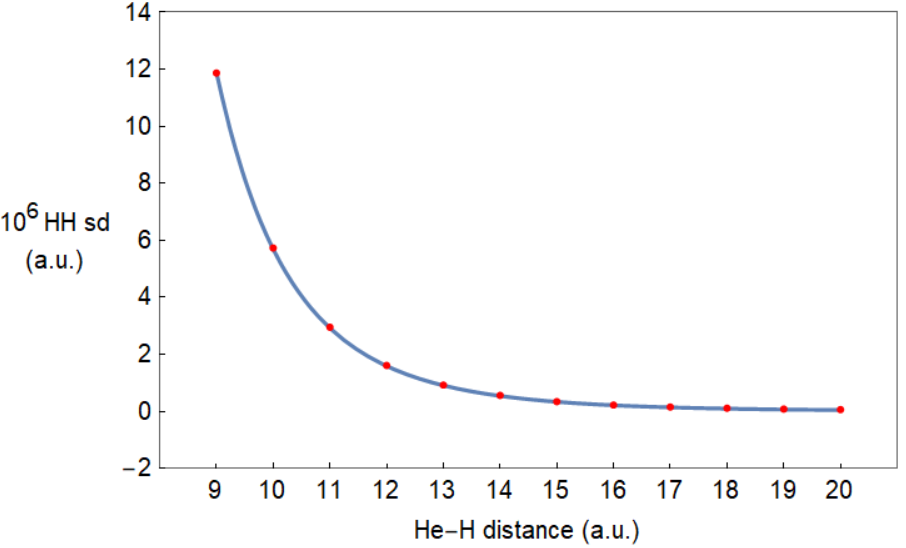
**Figure S37.** HeHe sg correlation charge density matrix elements fitted with R-7 with a.u. This plot is scaled by 106.



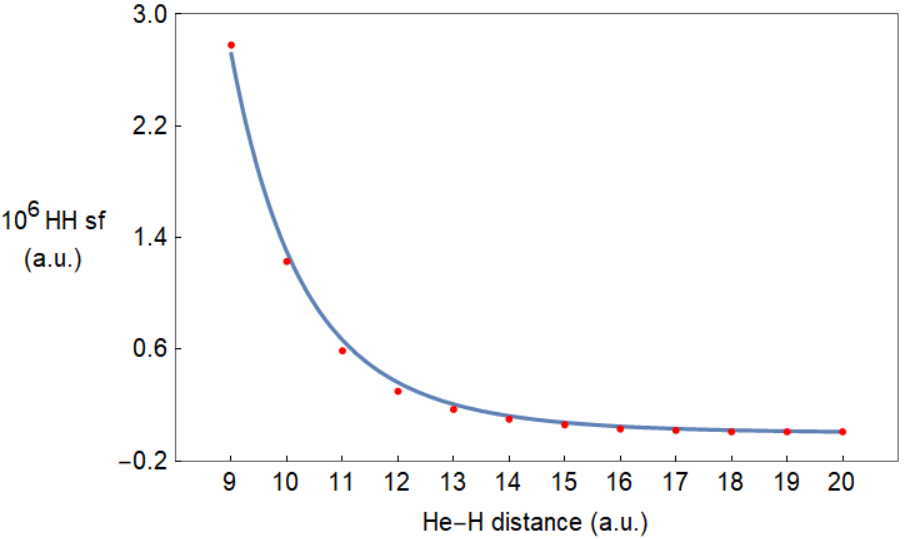
**Figure S38.** First HH sp correlation charge density matrix element in the list fitted with R-7, with a.u. This plot is scaled by 106.



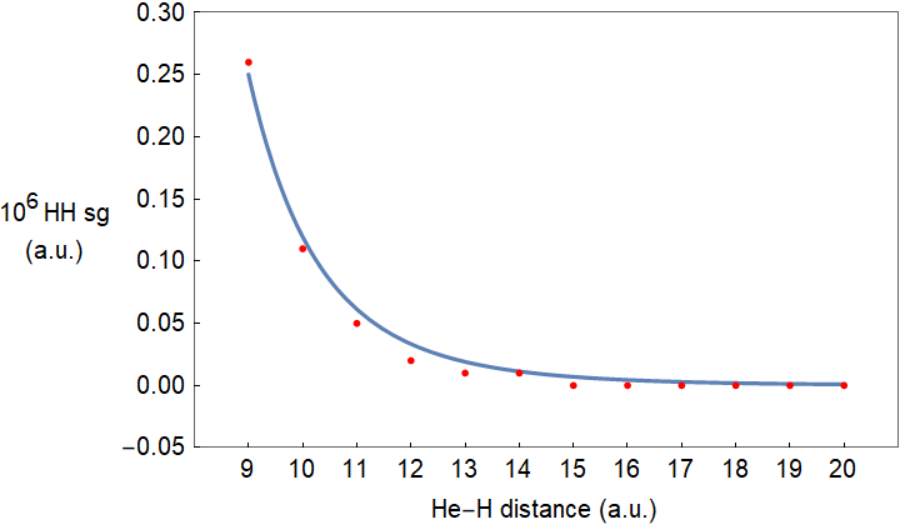
**Figure S39.** First HH sd correlation charge density matrix element in the list fitted with R-7, with a.u. This plot is scaled by 106.



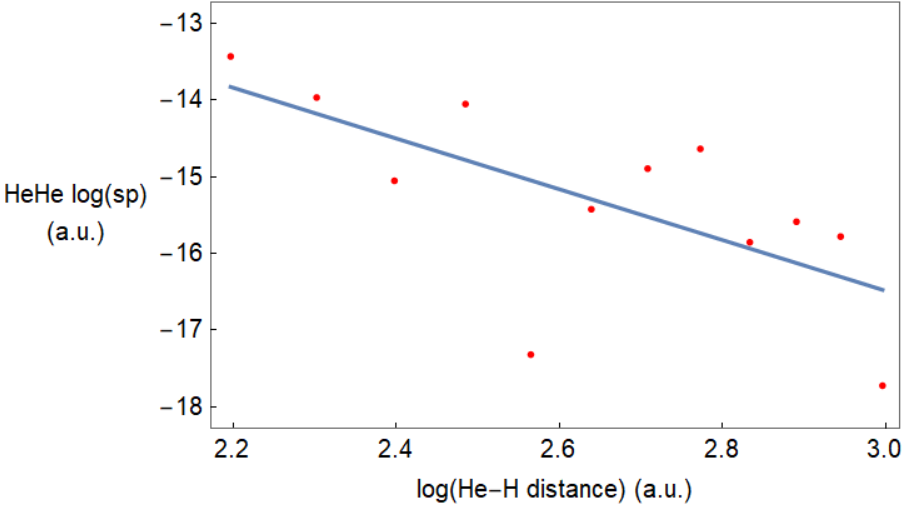
**Figure S40.** Second HH sd correlation charge density matrix element in the list fitted with R-7, with a.u. This plot is scaled by 106.



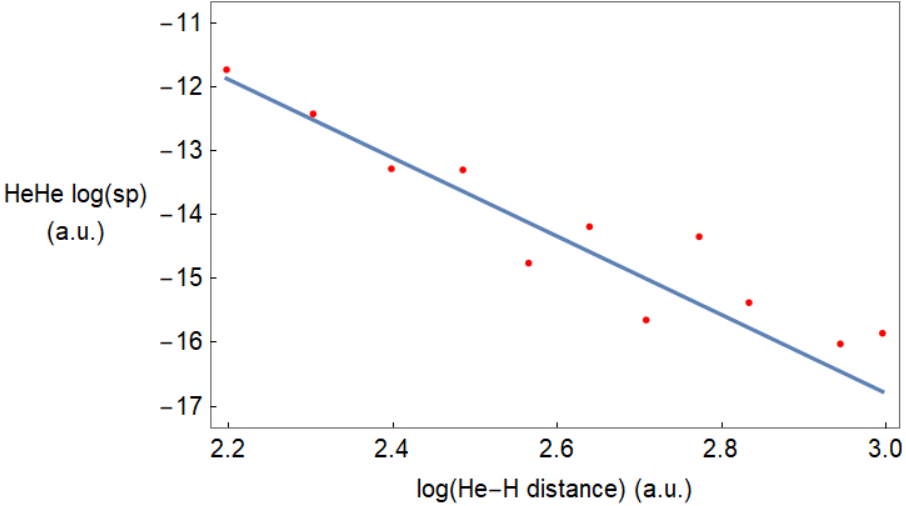
**Figure S41.** HH sf correlation charge density matrix elements fitted with R-7, with a.u. This plot is scaled by 106.



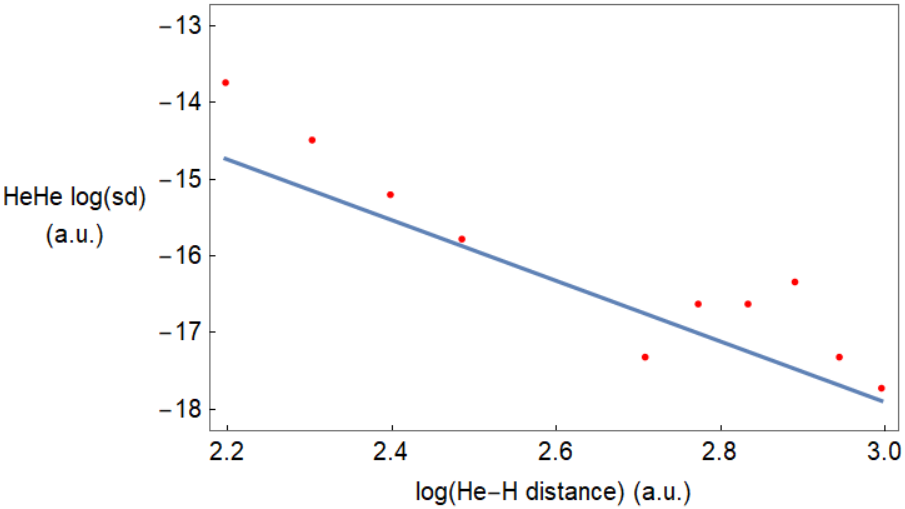
**Figure S42.** HH sg correlation charge density matrix elements fitted with R-7, with a.u. This plot is scaled by 106.



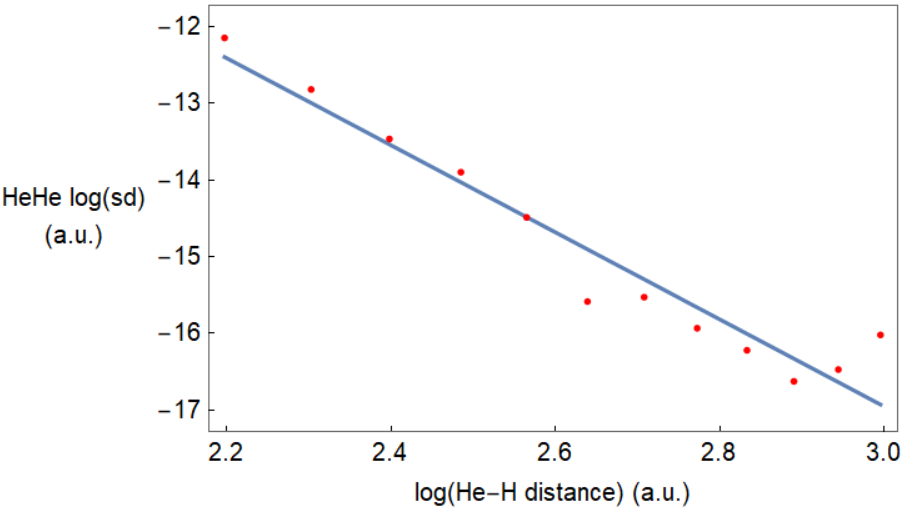
**Figure S43.** Log-Log plot of the first HeHe sp correlation charge density matrix element in the list fitted with a linear equation with a slope of -3.31706.



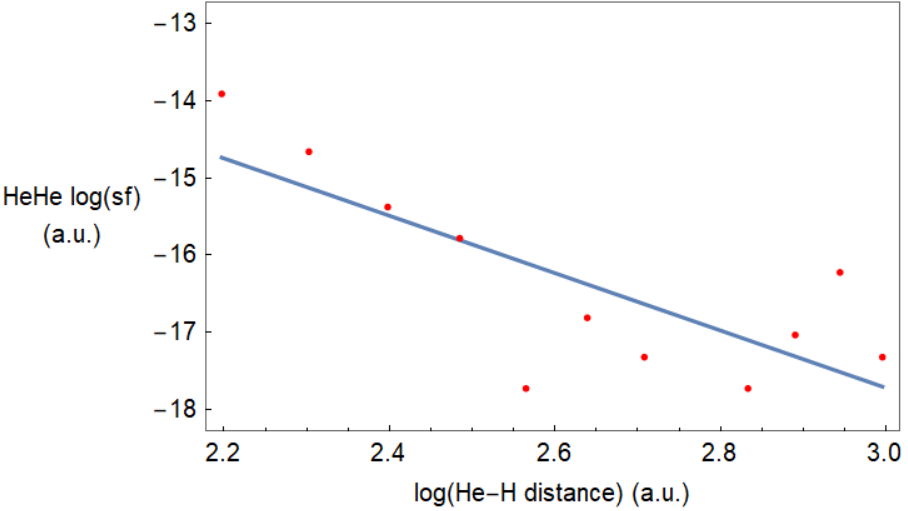
**Figure S44.** Log-Log plot of the second HeHe sp correlation charge density matrix element in the list fitted with a linear equation with a slope of -6.14168.



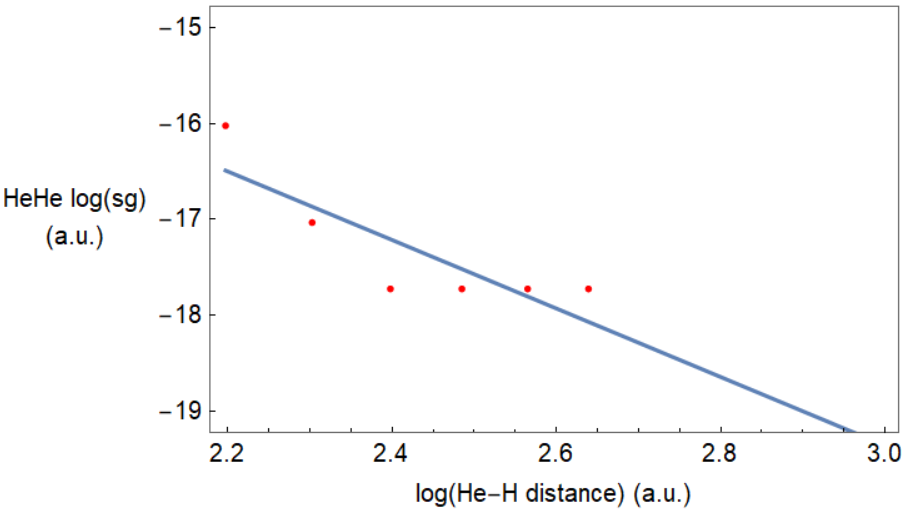
**Figure S45.** Log-Log plot of the first HeHe sd correlation charge density matrix element in the list fitted with a linear equation with a slope of -3.95717.



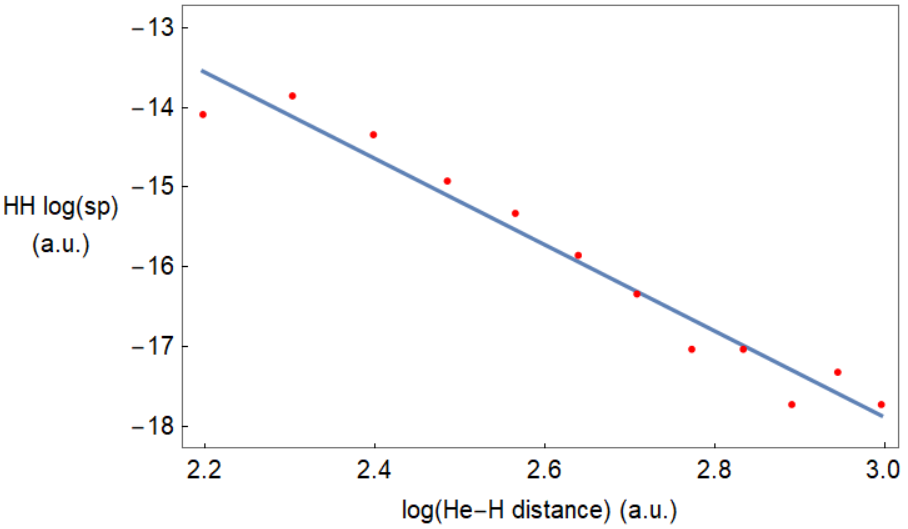
**Figure S46.** Log-Log plot of the second HeHe sd correlation charge density matrix element in the list fitted with a linear equation with a slope of -5.68068.



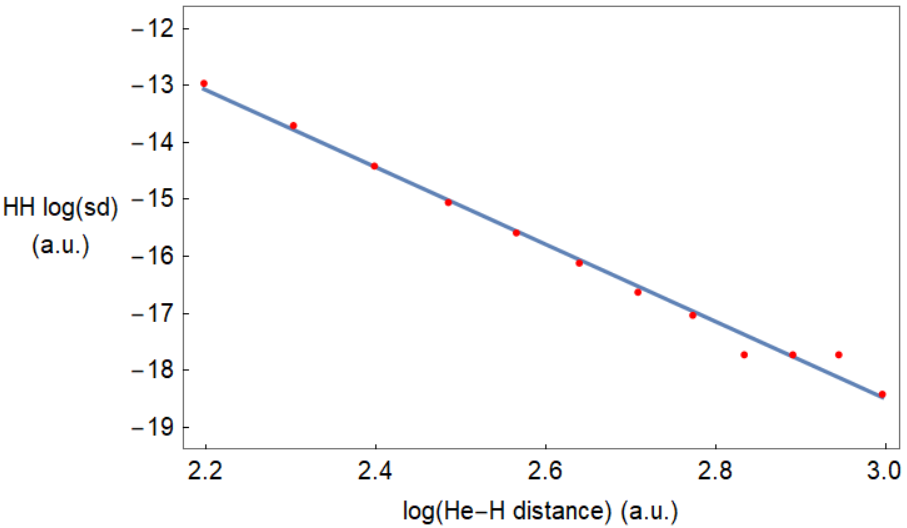
**Figure S47.** Log-Log plot of the HeHe sf correlation charge density matrix elements fitted with a linear equation with a slope of -3.71771. The correlation charge density matrix element at R = 15 a.u. is dropped from the fitting, due to log(0) is undefined.



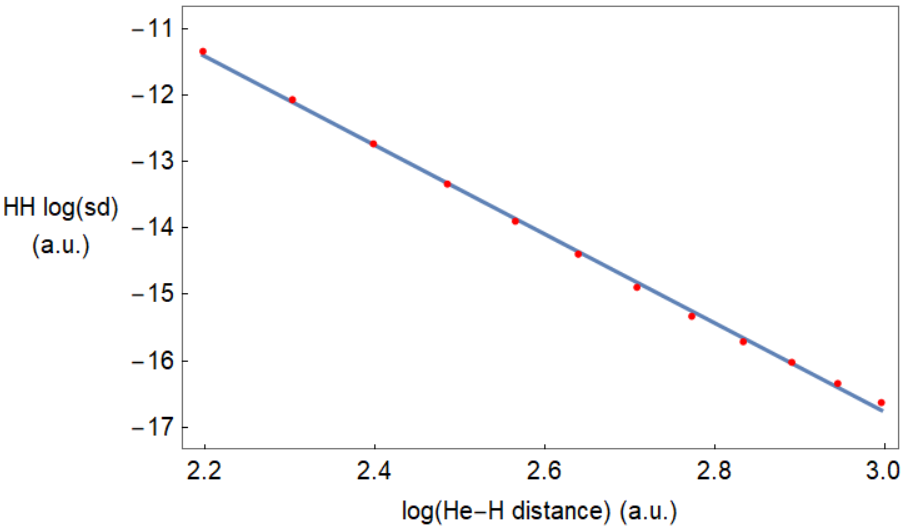
**Figure S48.** Log-Log plot of the HeHe sg correlation charge density matrix elements fitted with a linear equation with a slope of -3.576841. The correlation charge density matrix elements at R = 15 to 20 a.u. are dropped from the fitting, due to log(0) is undefined.



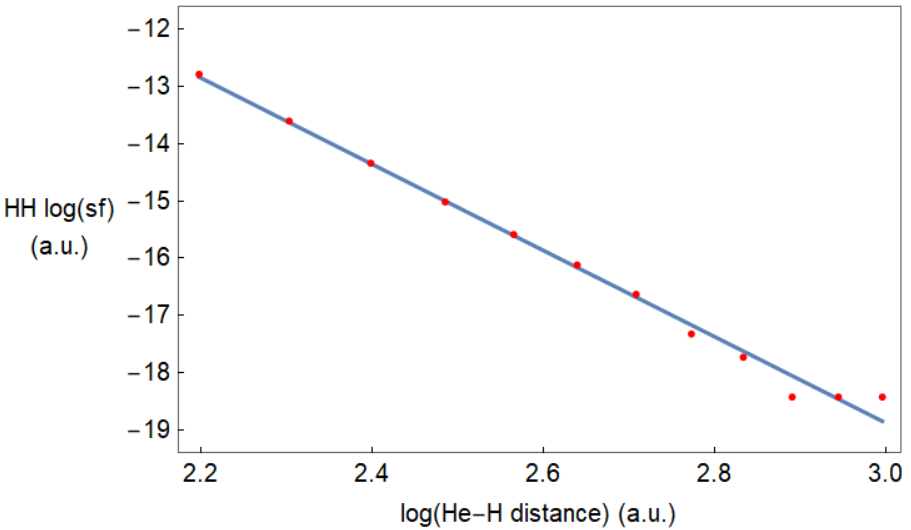
**Figure S49.** Log-Log plot of the first HH sp correlation charge density matrix element in the list fitted with a linear equation with a slope of -5.40815.



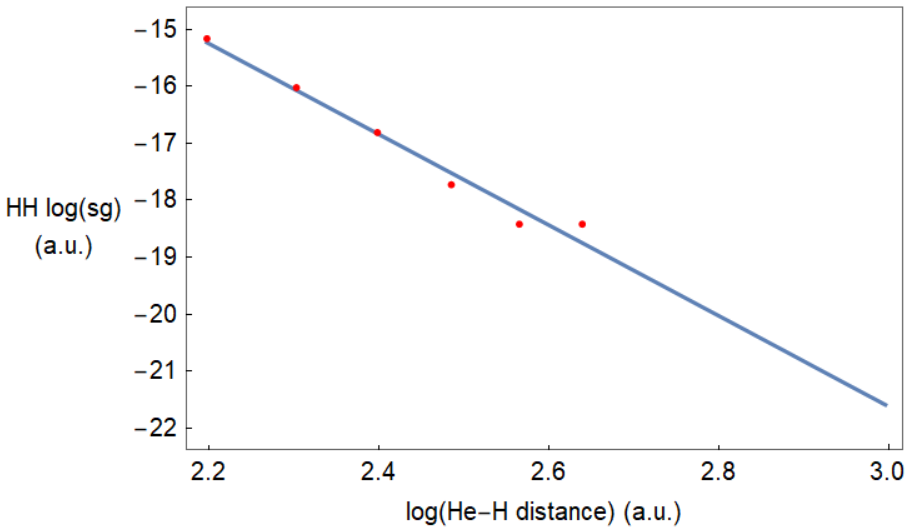
**Figure S50.** Log-Log plot of the first HH sd correlation charge density matrix element in the list fitted with a linear equation with a slope of -6.77712.



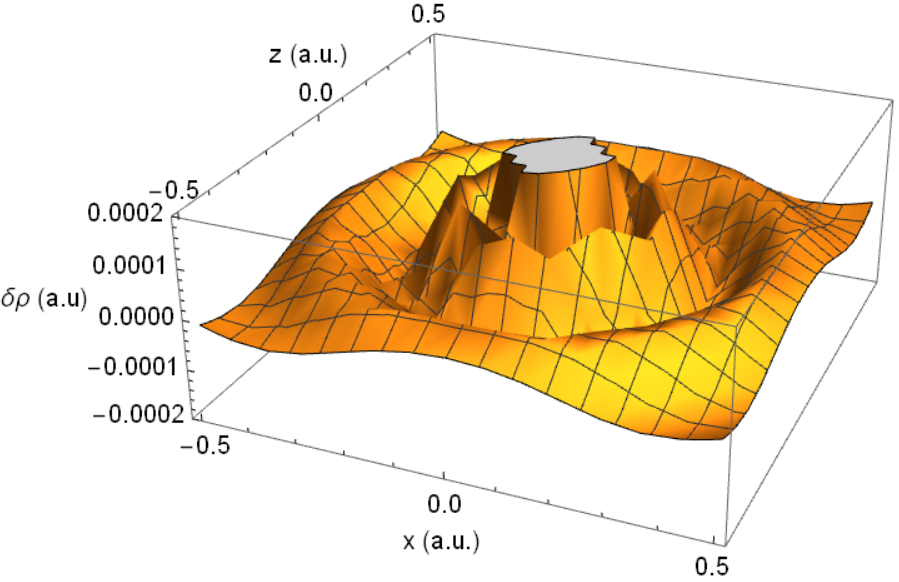
**Figure S51.** Log-Log plot of the second HH sd correlation charge density matrix element in the list fitted with a linear equation with a slope of -6.69034.



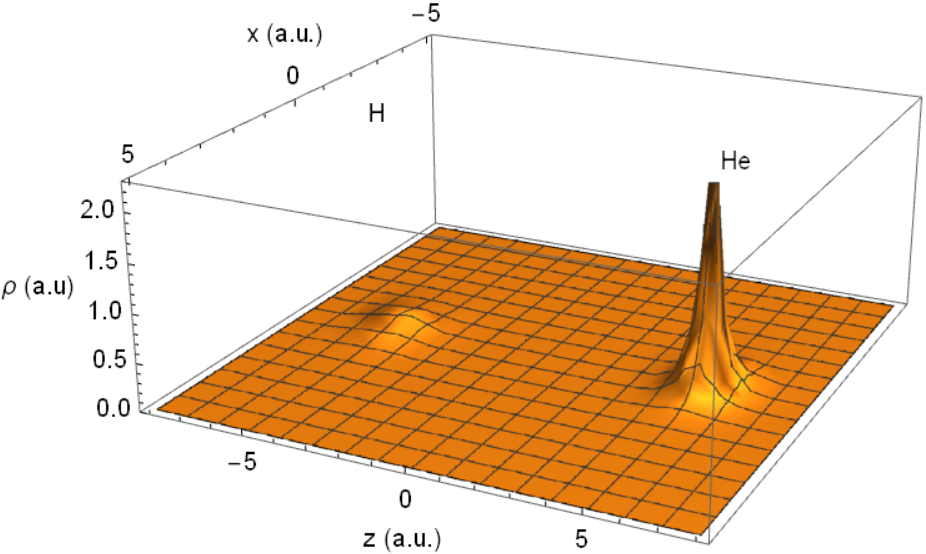
**Figure S52.** Log-Log plot of the HH sf correlation charge density matrix elements fitted with a linear equation with a slope of -7.51473



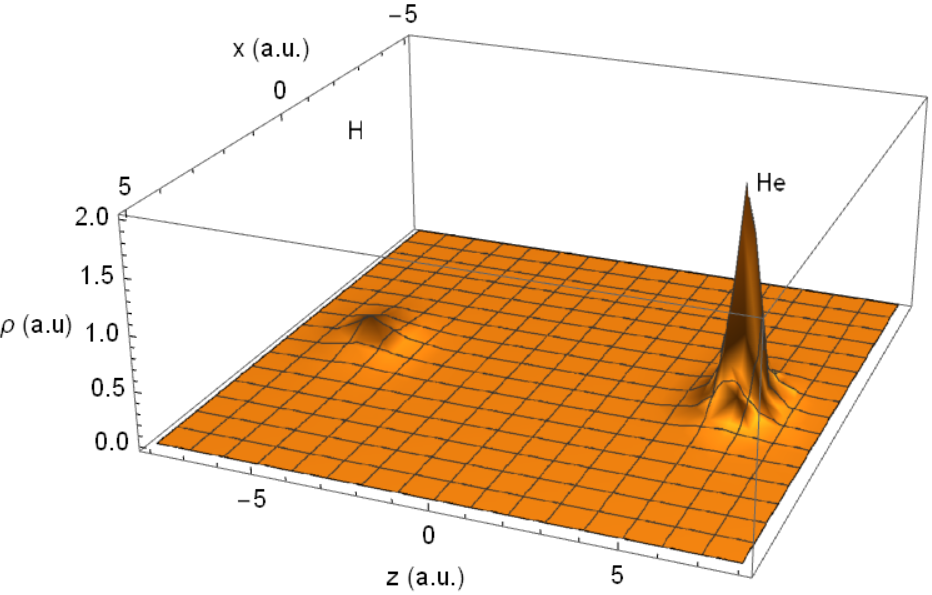
**Figure S53.** Log-Log plot of the HH sg correlation charge density matrix elements fitted with a linear equation with a slope of -7.9658.



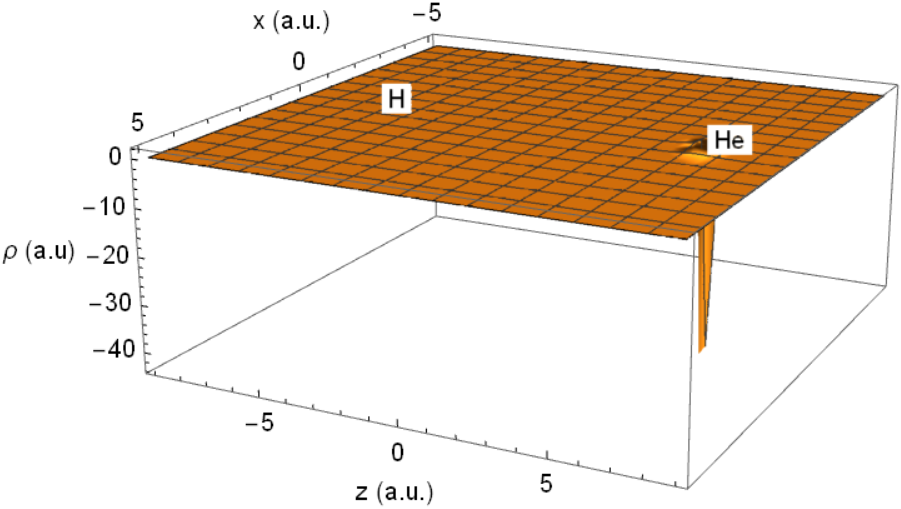
**Figure S54.** Enlargement of the difference of the charge density between the analytical expression and the calculated results from aug-cc-pV5Z level.



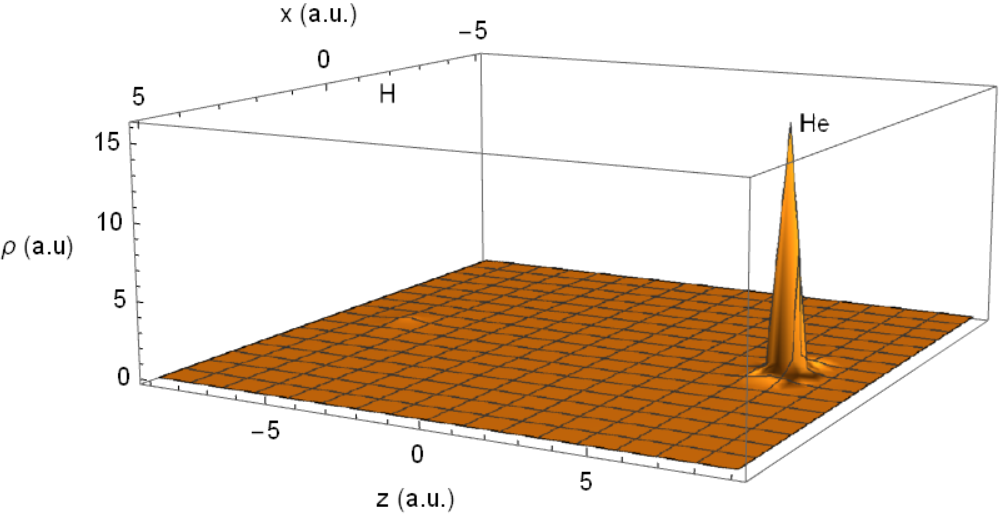
**Figure S55.** Calculated charge density of He-H system at separation R = 10 a.u.



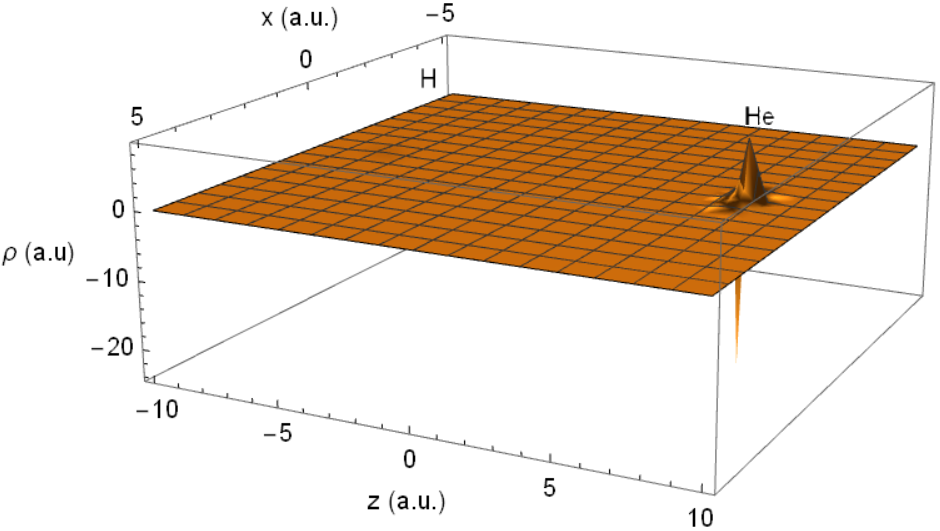
**Figure S56.** Calculated charge density of He-H system at separation R = 11 a.u.



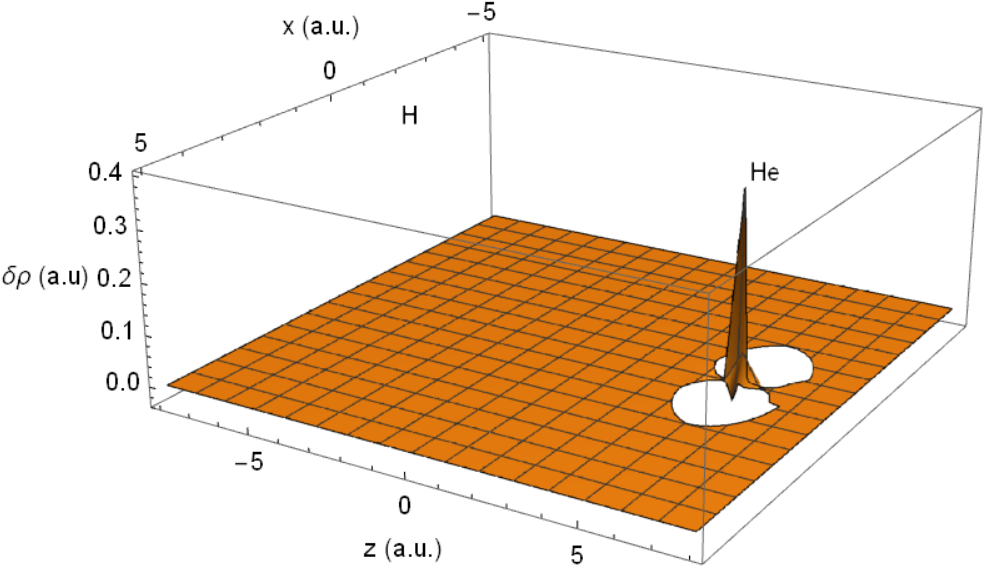
**Figure S57.** Calculated charge density of He-H system at separation R = 12 a.u.



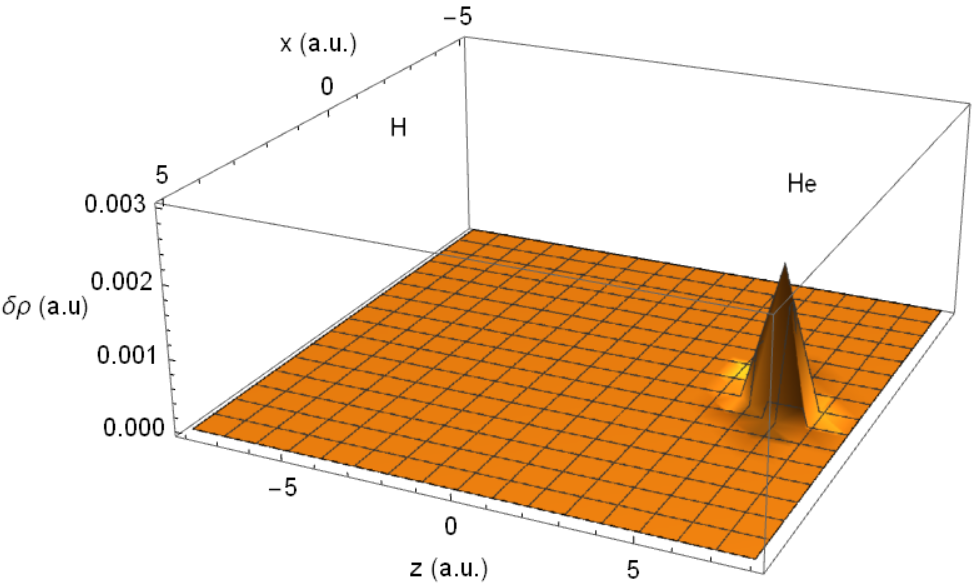
**Figure S58.** Calculated charge density of He-H system at separation R = 13 a.u.



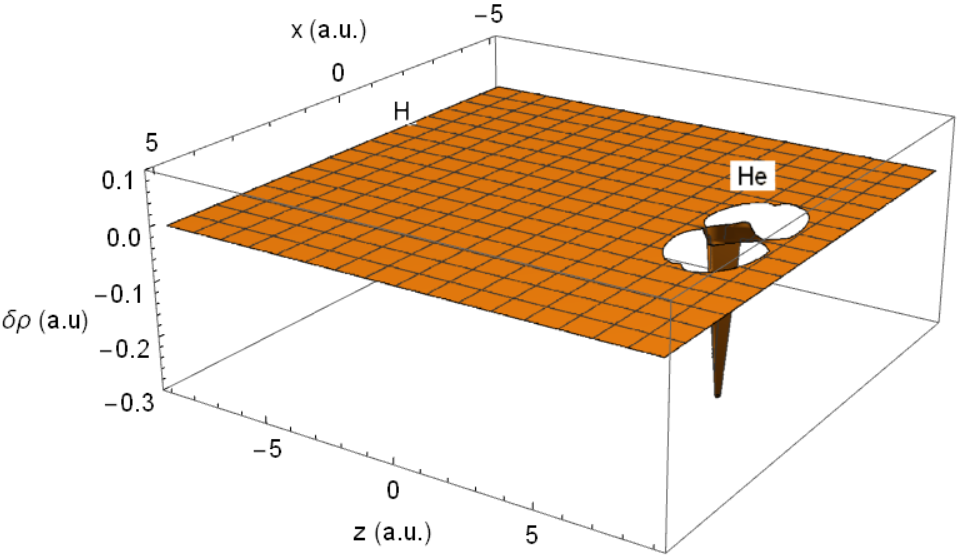
**Figure S59.** Calculated charge density of He-H system at separation R = 14 a.u.



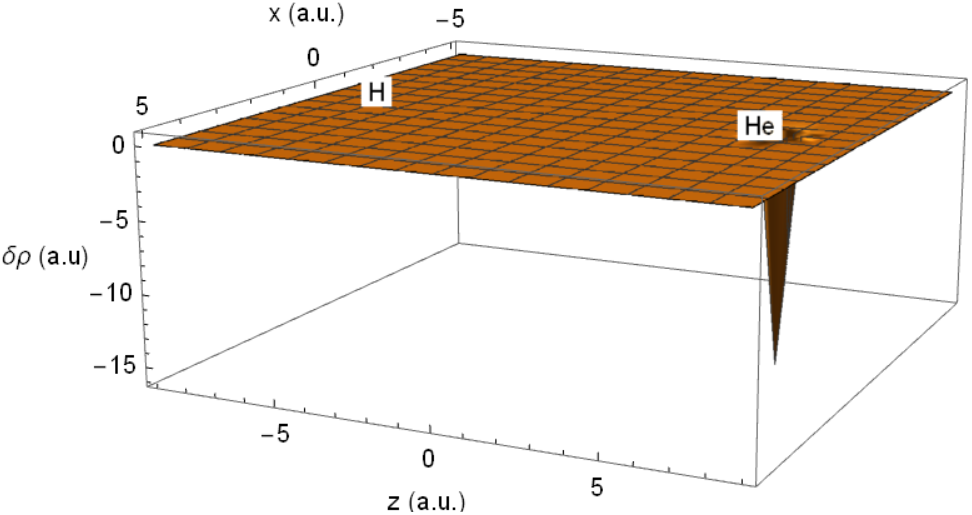
**Figure S60.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 10 a.u. The white area within the graph is due to the machine precision in Mathematica.



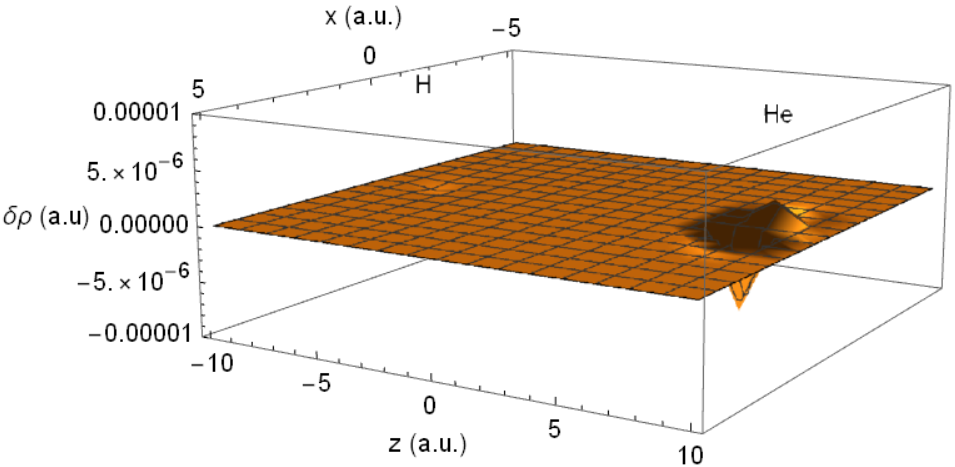
**Figure S61.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 11 a.u.



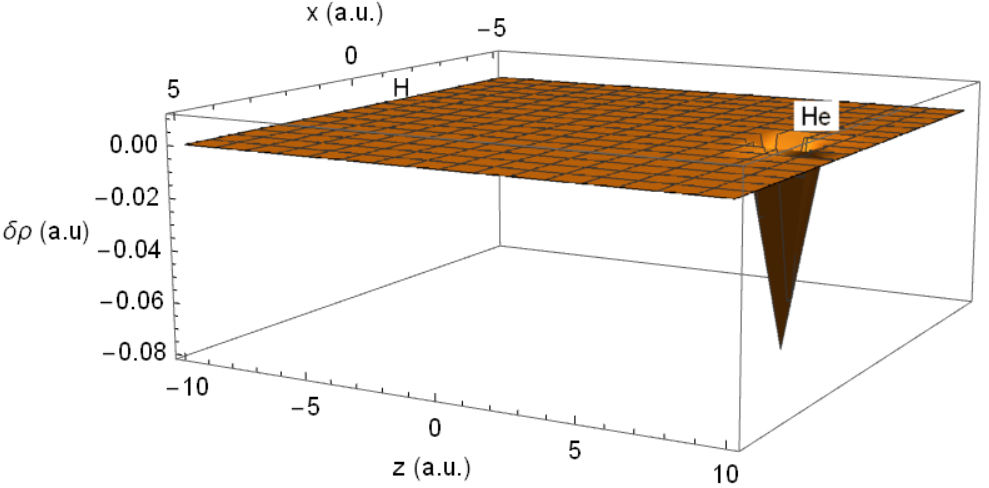
**Figure S62.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 12 a.u. The white area within the graph is due to the machine precision in Mathematica.



**Figure S63.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 13 a.u.



**Figure S64.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 14 a.u.



**Figure S65.** Change in charge density of He-H system at aug-cc-pV5Z and at separation R = 15 a.u.