

Supplementary material for “Electronic charge density distortions due to dispersion: Physically meaningful DMA multipoles for H₂, HeH, and He...He,” by Nathan D. Jansen, Hua-Kuang Lee, and Katharine L. C. Hunt

This supplement contains data tables for the figures in the article and ten additional figures. The quantities in all of the tables and all of the figures are given in atomic units.

Table S1. Energies of hydrogen in the triplet $b^3\Sigma_u^+$ state and in the ground singlet $X^1\Sigma_g^+$ state in the aug-cc-pV6Z basis, with R between 7.0 a.u. and 22.0 a.u.

Table S2. DMA dipole μ_z on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u. Results at RHF and full CI level are used to determine the correlation contribution.

Table S3. DMA dipole μ_z on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S4. DMA quadrupole Θ_{zz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S5. DMA quadrupole Θ_{zz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S6. DMA octopole Ω_{zzz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u. in the aug-cc-pV6Z basis.

Table S7. DMA octopole Ω_{zzz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S8. DMA hexadecapole Φ_{zzzz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S9. DMA hexadecapole Φ_{zzzz} on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S10. Total quadrupole Θ_{zz} relative to the center of symmetry for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S11. Total quadrupole Θ_{zz} relative to the center of symmetry for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S12. Total hexadecapole Φ_{zzzz} relative to the center of symmetry for the $b^3\Sigma_u^+$ state in the aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S13. Total hexadecapole Φ_{zzzz} relative to the center of symmetry for the $b^3\Sigma_u^+$ state in the d-aug-cc-pV6Z basis, with R between 5.0 a.u. and 22.0 a.u.

Table S14. Comparison of DMA dipoles μ_z on the H center at (0, 0, $-R/2$) for the $b^3\Sigma_u^+$ state in five basis sets: cc-pV6Z, aug-cc-pV5Z, aug-cc-pV6Z, d-aug-cc-pV5Z, and d-aug-cc-pV6Z.

Table S15. Dispersion charges associated with orbitals on a single center and overlap charges associated with orbitals on two centers, for the $b^3\Sigma_u^+$ state of H_2 , tabulated from 5.0 a.u. to 10.0 a.u. Since the net charges are identical in RHF and FCI calculations, the total charge should be zero, and differences from zero indicate numerical error.

Table S16. CAS(2,2) and FCI results for the energies, DMA dipoles, quadrupoles, octopoles, and hexadecapoles, and total quadrupoles and hexadecapoles for H_2 in the singlet state in the d-aug-cc-pV6Z basis, from $R = 12.0$ a.u. to 22.0 a.u.

Table S17. RHF and FCI results for the DMA dipoles of H and He and the total dipole of HeH in several different basis sets, from $R = 10.0$ a.u. to $R = 20.0$ a.u.

Table S18. Hartree-Fock and FCI results for the DMA dipoles of the He center at $(0, 0, -R/2)$ in $He\cdots He$ in the d-aug-cc-pV5Z basis, from $R = 8.0$ a.u. to $R = 20.0$ a.u.

Table S19. Number of configuration state functions and number of determinants in the FCI wave function for various basis sets.

Figure S1. Plot of the interaction energies of H_2 in the $b^3\Sigma_u^+$ state and the $X^1\Sigma_g^+$ state, from 10.0 a.u. to 22.0 a.u.

Figure S2. Plot of the dispersion charges associated with orbitals on a single center and overlap charges associated with orbitals on two centers, for the triplet state of H_2 , from 5.0 a.u. to 10.0 a.u. The total dispersion charge is very close to zero.

Figure S3. Energies of the $b^3\Sigma_u^+$ state of H_2 from this calculation compared with results in the literature, from 6.9 a.u. to 22.0 a.u.

Figure S4. Energies of the $X^1\Sigma_g^+$ state of H_2 from this calculation compared with results in the literature, from 7.0 a.u. to 11.0 a.u.

Figure S5. Dispersion energy of H_2 in the $X^1\Sigma_g^+$ state computed as the difference between the FCI energy and the CAS(2,2) energy in the d-aug-cc-pV6Z basis, compared with the long-range dispersion energy series including coefficients C_6 , C_8 , and C_{10} from Ref. 29.

Figure S6. Total dispersion quadrupole of H_2 in the $X^1\Sigma_g^+$ state in the d-aug-cc-pV6Z basis, compared with the long-range form from perturbation theory, with the same coefficients as found for the triplet state.

Figure S7. DMA dispersion octopole Ω_{zzz} on the H center at $(0, 0, -R/2)$ for the singlet state in the d-aug-cc-pV6Z basis.

Figure S8. DMA dispersion hexadecapole Φ_{zzzz} on the H center at $(0, 0, -R/2)$ for the singlet state in the d-aug-cc-pV6Z basis.

Figure S9. DMA dispersion dipole on the He center in HeH, in the range from $R = 10$ a.u. to $R = 20$ a.u., obtained with several different basis sets.

Figure S10. DMA dispersion dipole on the He center at $(0, 0, -R/2)$ in $He\cdots He$, in the range from $R = 12$ a.u. to 20 a.u., obtained with several different basis sets.

Table S1. Energies of hydrogen in the triplet state and in the ground singlet state

Energies at full configuration interaction level in the aug-cc-pV6Z basis are shown in a.u. To obtain the interaction energy, we have subtracted the energy at 22.0 a.u. in the triplet state (-0.99999861213714 a.u.) from the triplet state energies and we have subtracted the energy at 22.0 a.u. in the singlet state (-0.99999861213685 a.u.) from the singlet state energies. Then the energy at $R = 22.0$ a.u. equals zero in each state.

R (a.u.)	Triplet state E(FCI)	Singlet state E(FCI)
7.0	-1.00000102243249	-1.00019389185561
7.1	-1.00000595064625	-1.00016884691562
7.2	-1.00000975212659	-1.00014727943395
7.3	-1.00001262472952	-1.00012868968471
7.4	-1.00001473498140	-1.00011265056996
7.5	-1.00001622272054	-1.00009879708246
7.6	-1.00001720508558	-1.00008681727700
7.7	-1.00001777996615	-1.00007644454235
7.8	-1.00001802891250	-1.00006745099006
7.9	-1.00001801967929	-1.00005964180299
8.0	-1.00001780836902	-1.00005285040525
8.1	-1.00001744127440	-1.00004693433607
8.2	-1.00001695643955	-1.00004177171851
8.3	-1.00001638499364	-1.00003725828064
8.4	-1.00001575227818	-1.00003330473912
8.5	-1.00001507880351	-1.00002983463827
8.6	-1.00001438105754	-1.00002678247540
8.7	-1.00001367218630	-1.00002409206953
8.8	-1.00001296256990	-1.00002171526395
8.9	-1.00001226030362	-1.00001961069250
9.0	-1.00001157160432	-1.00001774282246
9.1	-1.00001090114940	-1.00001608110301
9.2	-1.00001025236076	-1.00001459923827
9.3	-1.00000962764175	-1.00001327457157
9.4	-1.00000902857440	-1.00001208756466
9.5	-1.00000845608370	-1.00001102134280
9.6	-1.00000791057335	-1.00001006131612
9.7	-1.00000739203790	-1.00000919485422
9.8	-1.00000690015498	-1.00000841100688
9.9	-1.00000643436133	-1.00000770026668
10.0	-1.00000599391409	-1.00000705436641
10.1	-1.00000557794109	-1.00000646610506
10.2	-1.00000518548102	-1.00000592919921
10.3	-1.00000481551587	-1.00000543815758

10.4	-1.00000446699630	-1.00000498817167
10.5	-1.00000413886183	-1.00000457502323
10.6	-1.00000383005640	-1.00000419500243
10.7	-1.00000353954018	-1.00000384484253
10.8	-1.00000326629858	-1.00000352165853
10.9	-1.00000300934866	-1.00000322289744
11.0	-1.00000276774376	-1.00000294629565
11.5	-1.00000175958915	-1.00000183236278
12.0	-1.00000101656346	-1.00000104610273
12.5	-1.00000046516910	-1.00000047710957
13.0	-1.00000005207871	-1.00000005688556
13.5	-0.99999973931567	-0.99999974124286
14.0	-0.99999950003110	-0.99999950080064
14.5	-0.99999931518463	-0.99999931549015
15.0	-0.99999917112282	-0.99999917124362
15.5	-0.99999905791468	-0.99999905796189
16.0	-0.99999896824401	-0.99999896826229
16.5	-0.99999889667019	-0.99999889667715
17.0	-0.99999883911965	-0.99999883912205
17.5	-0.99999879252327	-0.99999879252401
18.0	-0.99999875455234	-0.99999875455241
18.5	-0.99999872342527	-0.99999872342448
19.0	-0.99999869776680	-0.99999869776649
19.5	-0.99999867650590	-0.99999867650562
20.0	-0.99999865880220	-0.99999865880179
20.5	-0.99999864399108	-0.99999864399064
21.0	-0.99999863154429	-0.99999863154389
21.5	-0.99999862103945	-0.99999862103911
22.0	-0.99999861213714	-0.99999861213685

Table S2

Triplet	DMA Dipole μ_z		
	aug6z	aug6z	aug6z
R (a.u)	HF DMA μ_z	FCI DMA μ_z	Correlation
5.00	2.1207E-02	1.9564E-02	-1.6430E-03
5.50	1.1218E-02	9.9042E-03	-1.3138E-03
6.00	5.7813E-03	4.7939E-03	-9.8740E-04
6.50	2.9120E-03	2.2030E-03	-7.0900E-04
7.00	1.4369E-03	9.4412E-04	-4.9278E-04
7.50	6.9579E-04	3.6029E-04	-3.3550E-04
7.85	4.1438E-04	1.6013E-04	-2.5425E-04
8.00	3.3099E-04	1.0525E-04	-2.2574E-04
8.50	1.5469E-04	3.0424E-06	-1.5165E-04
9.00	7.0924E-05	-3.1328E-05	-1.0225E-04
9.50	3.1853E-05	-3.7693E-05	-6.9546E-05
10.00	1.4039E-05	-3.3786E-05	-4.7825E-05
10.50	6.0998E-06	-2.7275E-05	-3.3375E-05
11.00	2.5888E-06	-2.1027E-05	-2.3616E-05
11.50	9.9212E-07	-1.5980E-05	-1.6972E-05
12.00	2.2296E-07	-1.1951E-05	-1.2174E-05
12.50	-1.5252E-07	-9.0678E-06	-8.9153E-06
13.00	-3.0786E-07	-6.8883E-06	-6.5804E-06
13.50	-3.3245E-07	-5.4126E-06	-5.0802E-06
14.00	-2.8980E-07	-4.0992E-06	-3.8094E-06
14.50	-2.2588E-07	-3.1735E-06	-2.9476E-06
15.00	-1.6731E-07	-2.5351E-06	-2.3678E-06
15.50	-1.2379E-07	-1.9871E-06	-1.8633E-06
16.00	-9.4572E-08	-1.5253E-06	-1.4307E-06
16.50	-7.5015E-08	-1.2102E-06	-1.1352E-06
17.00	-6.0680E-08	-9.7956E-07	-9.1888E-07
17.50	-4.8841E-08	-7.9498E-07	-7.4614E-07
18.00	-3.8386E-08	-6.5477E-07	-6.1638E-07
18.50	-2.9145E-08	-5.4971E-07	-5.2057E-07
19.00	-2.1278E-08	-4.5088E-07	-4.2960E-07
19.50	-1.4916E-08	-3.4283E-07	-3.2791E-07
20.00	-1.0038E-08	-3.0051E-07	-2.9047E-07
20.50	-6.4831E-09	-2.5420E-07	-2.4772E-07
21.00	-4.0131E-09	-2.1650E-07	-2.1249E-07
21.50	-2.3731E-09	-1.9045E-07	-1.8808E-07
22.00	-1.3317E-09	-1.7246E-07	-1.7113E-07

Table S3

Triplet	DMA Dipole μ_z		
	daug6z	daug6z	daug6z
R (a.u)	HF DMA μ_z	FCI DMA μ_z	Correlation
5.00	2.1904E-02	2.0126E-02	-1.7780E-03
5.50	1.1523E-02	1.0090E-02	-1.4330E-03
6.00	5.8952E-03	4.8208E-03	-1.0744E-03
6.50	2.9527E-03	2.1848E-03	-7.6790E-04
7.00	1.4457E-03	9.1390E-04	-5.3180E-04
7.50	6.9276E-04	3.3150E-04	-3.6126E-04
7.85	4.0844E-04	1.3428E-04	-2.7416E-04
8.00	3.2464E-04	8.1479E-05	-2.4316E-04
8.50	1.5016E-04	-1.3995E-05	-1.6416E-04
9.00	7.1022E-05	-4.0476E-05	-1.1150E-04
9.50	3.5842E-05	-4.0704E-05	-7.6546E-05
10.00	1.9263E-05	-3.3827E-05	-5.3090E-05
10.50	1.0380E-05	-2.6878E-05	-3.7258E-05
11.00	5.1789E-06	-2.1286E-05	-2.6465E-05
11.50	2.1975E-06	-1.6853E-05	-1.9051E-05
12.00	6.4095E-07	-1.2991E-05	-1.3632E-05
12.50	-1.0321E-07	-1.0105E-05	-1.0002E-05
13.00	-4.5756E-07	-7.9411E-06	-7.4835E-06
13.50	-6.4016E-07	-6.3202E-06	-5.6800E-06
14.00	-7.2939E-07	-5.1180E-06	-4.3886E-06
14.50	-7.4453E-07	-4.0697E-06	-3.3252E-06
15.00	-6.9515E-07	-3.2661E-06	-2.5710E-06
15.50	-5.9710E-07	-2.6421E-06	-2.0450E-06
16.00	-4.7120E-07	-2.0987E-06	-1.6275E-06
16.50	-3.3771E-07	-1.6321E-06	-1.2944E-06
17.00	-2.1243E-07	-1.2456E-06	-1.0332E-06
17.50	-1.0530E-07	-9.4173E-07	-8.3643E-07
18.00	-2.0866E-08	-6.7785E-07	-6.5698E-07
18.50	4.0477E-08	-5.0279E-07	-5.4327E-07
19.00	8.1061E-08	-3.6190E-07	-4.4296E-07
19.50	1.0463E-07	-2.6191E-07	-3.6654E-07
20.00	1.1533E-07	-2.1847E-07	-3.3380E-07
20.50	1.1706E-07	-1.6904E-07	-2.8610E-07
21.00	1.1310E-07	-1.2161E-07	-2.3471E-07
21.50	1.0594E-07	-8.0548E-08	-1.8649E-07
22.00	9.7357E-08	-4.9368E-08	-1.4673E-07

Table S4

Triplet	DMA Quadrupole Θ_{zz}		
	aug6Z	aug6Z	aug6Z
R (a.u)	HF DMA Θ_{zz}	FCI DMA Θ_{zz}	Correlation
5.00	3.4144E-02	3.1341E-02	-2.8030E-03
5.50	1.9831E-02	1.7424E-02	-2.4070E-03
6.00	1.1147E-02	9.2174E-03	-1.9296E-03
6.50	6.1039E-03	4.6432E-03	-1.4607E-03
7.00	3.2692E-03	2.2116E-03	-1.0576E-03
7.50	1.7194E-03	9.7682E-04	-7.4258E-04
7.85	1.0874E-03	5.1462E-04	-5.7278E-04
8.00	8.9220E-04	3.8094E-04	-5.1126E-04
8.50	4.6050E-04	1.1251E-04	-3.4799E-04
9.00	2.4024E-04	4.7327E-06	-2.3551E-04
9.50	1.2877E-04	-3.0543E-05	-1.5931E-04
10.00	6.9948E-05	-3.8248E-05	-1.0820E-04
10.50	3.5436E-05	-3.8602E-05	-7.4038E-05
11.00	1.3162E-05	-3.8227E-05	-5.1389E-05
11.50	-9.4646E-07	-3.7233E-05	-3.6287E-05
12.00	-8.4366E-06	-3.4295E-05	-2.5858E-05
12.50	-1.0889E-05	-2.9961E-05	-1.9072E-05
13.00	-1.0269E-05	-2.4615E-05	-1.4346E-05
13.50	-8.3745E-06	-1.9380E-05	-1.1006E-05
14.00	-6.3799E-06	-1.4951E-05	-8.5711E-06
14.50	-4.7942E-06	-1.1539E-05	-6.7448E-06
15.00	-3.6816E-06	-9.0799E-06	-5.3983E-06
15.50	-2.9163E-06	-7.2867E-06	-4.3704E-06
16.00	-2.3519E-06	-5.9011E-06	-3.5492E-06
16.50	-1.8908E-06	-4.7462E-06	-2.8554E-06
17.00	-1.4890E-06	-3.9116E-06	-2.4226E-06
17.50	-1.1368E-06	-3.1228E-06	-1.9860E-06
18.00	-8.3743E-07	-2.4637E-06	-1.6263E-06
18.50	-5.9445E-07	-1.9339E-06	-1.3395E-06
19.00	-4.0674E-07	-1.5388E-06	-1.1321E-06
19.50	-2.6845E-07	-1.2266E-06	-9.5815E-07
20.00	-1.7099E-07	-9.8858E-07	-8.1759E-07
20.50	-1.0509E-07	-7.6351E-07	-6.5842E-07
21.00	-6.2226E-08	-6.2938E-07	-5.6715E-07
21.50	-3.5382E-08	-5.2584E-07	-4.9046E-07
22.00	-1.9194E-08	-4.3925E-07	-4.2006E-07

Table S5

Triplet R (a.u)	DMA Quadrupole Θ_{zz}		
	daug6Z HF DMA Θ_{zz}	daug6Z FCI DMA Θ_{zz}	daug6Z Correlation
5.00	3.7605E-02	3.4158E-02	-3.4470E-03
5.50	2.1500E-02	1.8482E-02	-3.0180E-03
6.00	1.1830E-02	9.4402E-03	-2.3898E-03
6.50	6.3759E-03	4.6106E-03	-1.7653E-03
7.00	3.3439E-03	2.1017E-03	-1.2422E-03
7.50	1.7101E-03	8.6574E-04	-8.4436E-04
7.85	1.0531E-03	4.1460E-04	-6.3850E-04
8.00	8.5317E-04	2.8642E-04	-5.6675E-04
8.50	4.3036E-04	4.8419E-05	-3.8194E-04
9.00	2.4493E-04	-1.5736E-05	-2.6067E-04
9.50	1.6874E-04	-1.1802E-05	-1.8054E-04
10.00	1.2920E-04	2.5735E-06	-1.2663E-04
10.50	9.7270E-05	7.3828E-06	-8.9887E-05
11.00	6.7496E-05	2.9924E-06	-6.4504E-05
11.50	4.2322E-05	-4.4488E-06	-4.6771E-05
12.00	2.4178E-05	-9.9886E-06	-3.4167E-05
12.50	1.3199E-05	-1.2129E-05	-2.5328E-05
13.00	7.7594E-06	-1.1319E-05	-1.9078E-05
13.50	5.6839E-06	-8.8684E-06	-1.4552E-05
14.00	5.1384E-06	-6.1386E-06	-1.1277E-05
14.50	4.9702E-06	-3.8574E-06	-8.8276E-06
15.00	4.6566E-06	-2.3156E-06	-6.9722E-06
15.50	4.0865E-06	-1.5024E-06	-5.5889E-06
16.00	3.3416E-06	-1.1345E-06	-4.4761E-06
16.50	2.5504E-06	-1.0726E-06	-3.6230E-06
17.00	1.8176E-06	-1.1468E-06	-2.9644E-06
17.50	1.2040E-06	-1.2359E-06	-2.4399E-06
18.00	7.3145E-07	-1.2465E-06	-1.9780E-06
18.50	3.9503E-07	-1.2334E-06	-1.6284E-06
19.00	1.7514E-07	-1.1720E-06	-1.3471E-06
19.50	4.6419E-08	-1.1033E-06	-1.1497E-06
20.00	-1.6507E-08	-9.5651E-07	-9.4000E-07
20.50	-3.5760E-08	-8.6302E-07	-8.2726E-07
21.00	-2.8870E-08	-7.3790E-07	-7.0903E-07
21.50	-8.6185E-09	-5.8192E-07	-5.7330E-07
22.00	1.6432E-08	-4.9386E-07	-5.1029E-07

Table S6

Triplet R (a.u)	DMA Octopole Ω_{zzz}		
	aug6Z HF DMA Ω_{zzz}	aug6Z FCI DMA Ω_{zzz}	aug6Z Correlation
5.00	6.9399E-02	6.5108E-02	-4.2910E-03
5.50	4.4016E-02	3.9841E-02	-4.1750E-03
6.00	2.6923E-02	2.3232E-02	-3.6910E-03
6.50	1.6043E-02	1.3037E-02	-3.0060E-03
7.00	9.3656E-03	7.0760E-03	-2.2896E-03
7.50	5.3829E-03	3.7208E-03	-1.6621E-03
7.85	3.6337E-03	2.3335E-03	-1.3002E-03
8.00	3.0698E-03	1.9048E-03	-1.1650E-03
8.50	1.7591E-03	9.6492E-04	-7.9418E-04
9.00	1.0282E-03	5.0071E-04	-5.2749E-04
9.50	6.1676E-04	2.7500E-04	-3.4176E-04
10.00	3.7041E-04	1.5413E-04	-2.1628E-04
10.50	2.0590E-04	7.1853E-05	-1.3405E-04
11.00	8.7834E-05	5.9481E-06	-8.1886E-05
11.50	6.7423E-06	-4.3000E-05	-4.9742E-05
12.00	-3.9806E-05	-6.9560E-05	-2.9754E-05
12.50	-5.7502E-05	-7.6076E-05	-1.8574E-05
13.00	-5.6145E-05	-6.8345E-05	-1.2200E-05
13.50	-4.5913E-05	-5.4050E-05	-8.1370E-06
14.00	-3.4135E-05	-3.9879E-05	-5.7440E-06
14.50	-2.4454E-05	-2.8684E-05	-4.2300E-06
15.00	-1.7727E-05	-2.0913E-05	-3.1860E-06
15.50	-1.3402E-05	-1.5861E-05	-2.4590E-06
16.00	-1.0579E-05	-1.2506E-05	-1.9270E-06
16.50	-8.5372E-06	-1.0061E-05	-1.5238E-06
17.00	-6.8666E-06	-8.0862E-06	-1.2196E-06
17.50	-5.4044E-06	-6.3901E-06	-9.8570E-07
18.00	-4.1212E-06	-4.9242E-06	-8.0300E-07
18.50	-3.0325E-06	-3.6892E-06	-6.5670E-07
19.00	-2.1512E-06	-2.6933E-06	-5.4210E-07
19.50	-1.4717E-06	-1.9222E-06	-4.5050E-07
20.00	-9.7158E-07	-1.3472E-06	-3.7562E-07
20.50	-6.1889E-07	-9.3323E-07	-3.1434E-07
21.00	-3.7993E-07	-6.4404E-07	-2.6411E-07
21.50	-2.2408E-07	-4.4760E-07	-2.2352E-07
22.00	-1.2617E-07	-3.1685E-07	-1.9068E-07

Table S7

Triplet	DMA Octopole Ω_{zzz}		
	daug6Z	daug6Z	daug6Z
R (a.u)	HF DMA Ω_{zzz}	FCI DMA Ω_{zzz}	Correlation
5.00	8.0381E-02	7.3610E-02	-6.7710E-03
5.50	5.0294E-02	4.3543E-02	-6.7510E-03
6.00	2.9841E-02	2.4012E-02	-5.8290E-03
6.50	1.7164E-02	1.2610E-02	-4.5540E-03
7.00	9.5179E-03	6.2321E-03	-3.2858E-03
7.50	5.1109E-03	2.8908E-03	-2.2201E-03
7.85	3.2333E-03	1.5855E-03	-1.6478E-03
8.00	2.6463E-03	1.2002E-03	-1.4461E-03
8.50	1.4076E-03	4.6947E-04	-9.3813E-04
9.00	9.3382E-04	3.1693E-04	-6.1689E-04
9.50	8.0475E-04	3.9133E-04	-4.1342E-04
10.00	7.3050E-04	4.4873E-04	-2.8177E-04
10.50	6.0222E-04	4.0779E-04	-1.9443E-04
11.00	4.2965E-04	2.9475E-04	-1.3490E-04
11.50	2.5863E-04	1.6499E-04	-9.3640E-05
12.00	1.2261E-04	5.7506E-05	-6.5104E-05
12.50	3.1217E-05	-1.4448E-05	-4.5665E-05
13.00	-2.1513E-05	-5.4035E-05	-3.2522E-05
13.50	-4.6632E-05	-7.0106E-05	-2.3474E-05
14.00	-5.4374E-05	-7.1480E-05	-1.7106E-05
14.50	-5.2312E-05	-6.5028E-05	-1.2716E-05
15.00	-4.5419E-05	-5.5027E-05	-9.6080E-06
15.50	-3.6695E-05	-4.4004E-05	-7.3090E-06
16.00	-2.7830E-05	-3.3500E-05	-5.6700E-06
16.50	-1.9708E-05	-2.4225E-05	-4.5170E-06
17.00	-1.2748E-05	-1.6326E-05	-3.5780E-06
17.50	-7.0992E-06	-9.9017E-06	-2.8025E-06
18.00	-2.7477E-06	-4.9889E-06	-2.2412E-06
18.50	4.2111E-07	-1.4096E-06	-1.8307E-06
19.00	2.5824E-06	1.0745E-06	-1.5079E-06
19.50	3.9380E-06	2.7083E-06	-1.2297E-06
20.00	4.6891E-06	3.6976E-06	-9.9150E-07
20.50	5.0165E-06	4.2471E-06	-7.6940E-07
21.00	5.0693E-06	4.4238E-06	-6.4550E-07
21.50	4.9611E-06	4.4191E-06	-5.4200E-07
22.00	4.7716E-06	4.3147E-06	-4.5690E-07

Table S8

Triplet	DMA Hexadecapole Φ_{zzzz}		
	aug6z	aug6z	aug6z
R (a.u)	HF DMA Φ_{zzzz}	FCI DMA Φ_{zzzz}	Correlation
5.00	1.5471E-01	1.4533E-01	-9.3800E-03
5.50	1.0705E-01	9.7119E-02	-9.9310E-03
6.00	7.1261E-02	6.1816E-02	-9.4450E-03
6.50	4.6144E-02	3.7938E-02	-8.2060E-03
7.00	2.9173E-02	2.2537E-02	-6.6360E-03
7.50	1.8076E-02	1.2972E-02	-5.1040E-03
7.85	1.2832E-02	8.6781E-03	-4.1539E-03
8.00	1.1071E-02	7.2873E-03	-3.7837E-03
8.50	6.7877E-03	4.0713E-03	-2.7164E-03
9.00	4.2304E-03	2.3464E-03	-1.8840E-03
9.50	2.7053E-03	1.4449E-03	-1.2604E-03
10.00	1.7403E-03	9.2875E-04	-8.1155E-04
10.50	1.0478E-03	5.4594E-04	-5.0186E-04
11.00	5.0178E-04	2.0373E-04	-2.9805E-04
11.50	8.5723E-05	-8.4232E-05	-1.6996E-04
12.00	-1.8197E-04	-2.7293E-04	-9.0960E-05
12.50	-3.0332E-04	-3.5171E-04	-4.8390E-05
13.00	-3.1320E-04	-3.3884E-04	-2.5640E-05
13.50	-2.6168E-04	-2.7539E-04	-1.3710E-05
14.00	-1.9223E-04	-1.9944E-04	-7.2100E-06
14.50	-1.3093E-04	-1.3487E-04	-3.9400E-06
15.00	-8.7266E-05	-8.9547E-05	-2.2810E-06
15.50	-6.0242E-05	-6.1643E-05	-1.4010E-06
16.00	-4.4784E-05	-4.5730E-05	-9.4600E-07
16.50	-3.5758E-05	-3.6404E-05	-6.4600E-07
17.00	-2.9620E-05	-3.0074E-05	-4.5400E-07
17.50	-2.4533E-05	-2.4862E-05	-3.2900E-07
18.00	-1.9843E-05	-2.0092E-05	-2.4900E-07
18.50	-1.5503E-05	-1.5689E-05	-1.8600E-07
19.00	-1.1656E-05	-1.1802E-05	-1.4600E-07
19.50	-8.4315E-06	-8.5483E-06	-1.1680E-07
20.00	-5.8717E-06	-5.9653E-06	-9.3600E-08
20.50	-3.9382E-06	-4.0142E-06	-7.6000E-08
21.00	-2.5419E-06	-2.5991E-06	-5.7200E-08
21.50	-1.5745E-06	-1.6207E-06	-4.6200E-08
22.00	-9.3035E-07	-9.7572E-07	-4.5370E-08

Table S9

Triplet	DMA Hexadecapole Φ_{zzzz}		
	daug6Z	daug6Z	daug6Z
R (a.u)	HF DMA Φ_{zzzz}	FCI DMA Φ_{zzzz}	Correlation
5.00	1.7784E-01	1.6085E-01	-1.6990E-02
5.50	1.2655E-01	1.0805E-01	-1.8500E-02
6.00	8.3351E-02	6.5816E-02	-1.7535E-02
6.50	5.1250E-02	3.6345E-02	-1.4905E-02
7.00	2.9928E-02	1.8484E-02	-1.1444E-02
7.50	1.6943E-02	8.9271E-03	-8.0159E-03
7.85	1.1145E-02	5.1370E-03	-6.0080E-03
8.00	9.2958E-03	4.0257E-03	-5.2701E-03
8.50	5.5026E-03	2.1220E-03	-3.3806E-03
9.00	4.5213E-03	2.3568E-03	-2.1645E-03
9.50	4.7834E-03	3.3792E-03	-1.4042E-03
10.00	4.9379E-03	4.0146E-03	-9.2330E-04
10.50	4.4520E-03	3.8374E-03	-6.1460E-04
11.00	3.4427E-03	3.0330E-03	-4.0970E-04
11.50	2.2593E-03	1.9894E-03	-2.6990E-04
12.00	1.1971E-03	1.0205E-03	-1.7660E-04
12.50	4.0309E-04	2.8819E-04	-1.1490E-04
13.00	-1.0067E-04	-1.7350E-04	-7.2830E-05
13.50	-3.6215E-04	-4.0904E-04	-4.6890E-05
14.00	-4.5377E-04	-4.8498E-04	-3.1210E-05
14.50	-4.4394E-04	-4.6494E-04	-2.1000E-05
15.00	-3.8414E-04	-3.9817E-04	-1.4030E-05
15.50	-3.0696E-04	-3.1699E-04	-1.0030E-05
16.00	-2.3003E-04	-2.3710E-04	-7.0700E-06
16.50	-1.6144E-04	-1.6692E-04	-5.4800E-06
17.00	-1.0403E-04	-1.0816E-04	-4.1300E-06
17.50	-5.8141E-05	-6.1319E-05	-3.1780E-06
18.00	-2.2981E-05	-2.5445E-05	-2.4640E-06
18.50	2.7592E-06	8.3659E-07	-1.9226E-06
19.00	2.0629E-05	1.9375E-05	-1.2540E-06
19.50	3.2245E-05	3.1026E-05	-1.2190E-06
20.00	3.9156E-05	3.8401E-05	-7.5500E-07
20.50	4.2745E-05	4.1955E-05	-7.9000E-07
21.00	4.4152E-05	4.3888E-05	-2.6400E-07
21.50	4.4258E-05	4.4038E-05	-2.2000E-07
22.00	4.3690E-05	4.3512E-05	-1.7800E-07

Table S10

Triplet	Total Quadrupole Θ_{zz}		
	aug6Z	aug6Z	aug6Z
R (a.u.)	HF Θ_{zz} Tot	FCI Θ_{zz} Tot	Correlation
5.00	-1.4378E-01	-1.3296E-01	1.0820E-02
5.50	-8.3733E-02	-7.4098E-02	9.6350E-03
6.00	-4.7082E-02	-3.9091E-02	7.9910E-03
6.50	-2.5649E-02	-1.9352E-02	6.2970E-03
7.00	-1.3578E-02	-8.7944E-03	4.7836E-03
7.50	-6.9980E-03	-3.4507E-03	3.5473E-03
7.85	-4.3310E-03	-1.4848E-03	2.8462E-03
8.00	-3.5114E-03	-9.2218E-04	2.5892E-03
8.50	-1.7087E-03	1.7329E-04	1.8820E-03
9.00	-7.9615E-04	5.7337E-04	1.3695E-03
9.50	-3.4767E-04	6.5508E-04	1.0028E-03
10.00	-1.4088E-04	5.9922E-04	7.4010E-04
10.50	-5.7223E-05	4.9558E-04	5.5280E-04
11.00	-3.0630E-05	3.8614E-04	4.1677E-04
11.50	-2.4712E-05	2.9306E-04	3.1777E-04
12.00	-2.2224E-05	2.1823E-04	2.4045E-04
12.50	-1.7964E-05	1.6677E-04	1.8473E-04
13.00	-1.2533E-05	1.2987E-04	1.4240E-04
13.50	-7.7728E-06	1.0738E-04	1.1515E-04
14.00	-4.6454E-06	8.4874E-05	8.9519E-05
14.50	-3.0379E-06	6.8955E-05	7.1993E-05
15.00	-2.3438E-06	5.7893E-05	6.0237E-05
15.50	-1.9950E-06	4.7027E-05	4.9022E-05
16.00	-1.6775E-06	3.7006E-05	3.8684E-05
16.50	-1.3060E-06	3.0444E-05	3.1750E-05
17.00	-9.1488E-07	2.5482E-05	2.6397E-05
17.50	-5.6414E-07	2.1578E-05	2.2142E-05
18.00	-2.9297E-07	1.8644E-05	1.8937E-05
18.50	-1.1055E-07	1.6471E-05	1.6582E-05
19.00	-4.8986E-09	1.4056E-05	1.4061E-05
19.50	4.4854E-08	1.0917E-05	1.0872E-05
20.00	5.9553E-08	1.0043E-05	9.9834E-06
20.50	5.5640E-08	8.8953E-06	8.8397E-06
21.00	4.4094E-08	7.8343E-06	7.7902E-06
21.50	3.1282E-08	7.1375E-06	7.1062E-06
22.00	2.0202E-08	6.7096E-06	6.6894E-06

Table S11

Triplet	Total Quadrupole Θ_{zz}		
	daug6Z	daug6Z	daug6Z
R (a.u.)	HF Θ_{zz} Tot	FCI Θ_{zz} Tot	Correlation
5.00	-1.4383E-01	-1.3294E-01	1.0890E-02
5.50	-8.3757E-02	-7.4032E-02	9.7250E-03
6.00	-4.7083E-02	-3.8970E-02	8.1130E-03
6.50	-2.5633E-02	-1.9182E-02	6.4510E-03
7.00	-1.3552E-02	-8.5911E-03	4.9609E-03
7.50	-6.9712E-03	-3.2408E-03	3.7304E-03
7.85	-4.3063E-03	-1.2790E-03	3.0273E-03
8.00	-3.4879E-03	-7.3098E-04	2.7569E-03
8.50	-1.6920E-03	3.3513E-04	2.0271E-03
9.00	-7.8854E-04	6.9708E-04	1.4856E-03
9.50	-3.4351E-04	7.4969E-04	1.0932E-03
10.00	-1.2685E-04	6.8162E-04	8.0847E-04
10.50	-2.3443E-05	5.7909E-04	6.0253E-04
11.00	2.1056E-05	4.7457E-04	4.5351E-04
11.50	3.4102E-05	3.7864E-04	3.4454E-04
12.00	3.2973E-05	2.9283E-04	2.5986E-04
12.50	2.8979E-05	2.2838E-04	1.9940E-04
13.00	2.7416E-05	1.8382E-04	1.5640E-04
13.50	2.8652E-05	1.5293E-04	1.2428E-04
14.00	3.0700E-05	1.2942E-04	9.8720E-05
14.50	3.1532E-05	1.1021E-04	7.8678E-05
15.00	3.0168E-05	9.3348E-05	6.3180E-05
15.50	2.6683E-05	7.9068E-05	5.2385E-05
16.00	2.1762E-05	6.4681E-05	4.2919E-05
16.50	1.6245E-05	5.1690E-05	3.5445E-05
17.00	1.0858E-05	3.9952E-05	2.9094E-05
17.50	6.0934E-06	3.0305E-05	2.4212E-05
18.00	2.2141E-06	2.2344E-05	2.0130E-05
18.50	-7.0760E-07	1.6099E-05	1.6807E-05
19.00	-2.7300E-06	1.1370E-05	1.4100E-05
19.50	-3.9876E-06	8.6630E-06	1.2651E-05
20.00	-4.6462E-06	6.4417E-06	1.1088E-05
20.50	-4.8711E-06	5.2990E-06	1.0170E-05
21.00	-4.8078E-06	3.5924E-06	8.4002E-06
21.50	-4.5726E-06	2.3234E-06	6.8960E-06
22.00	-4.2508E-06	1.1150E-06	5.3658E-06

Table S12

Triplet R (a.u.)	Total Hexadecapole Φ_{zzzz}		
	aug6Z HF Φ_{zzzz} Tot	aug6Z FCI Φ_{zzzz} Tot	aug6Z Correlation
5.00	-1.1686E+00	-1.1064E+00	6.2200E-02
5.50	-8.2093E-01	-7.4882E-01	7.2110E-02
6.00	-5.4854E-01	-4.7392E-01	7.4620E-02
6.50	-3.5088E-01	-2.7955E-01	7.1330E-02
7.00	-2.1617E-01	-1.5178E-01	6.4390E-02
7.50	-1.2872E-01	-7.2841E-02	5.5879E-02
7.85	-8.7858E-02	-3.8240E-02	4.9618E-02
8.00	-7.4254E-02	-2.7127E-02	4.7127E-02
8.50	-4.1421E-02	-2.1470E-03	3.9274E-02
9.00	-2.1879E-02	1.0656E-02	3.2535E-02
9.50	-1.0472E-02	1.6487E-02	2.6959E-02
10.00	-4.3903E-03	1.8004E-02	2.2394E-02
10.50	-1.8931E-03	1.6881E-02	1.8774E-02
11.00	-1.5289E-03	1.4256E-02	1.5785E-02
11.50	-2.0231E-03	1.1340E-02	1.3363E-02
12.00	-2.4831E-03	8.6285E-03	1.1112E-02
12.50	-2.5376E-03	6.7668E-03	9.3044E-03
13.00	-2.2368E-03	5.5303E-03	7.7671E-03
13.50	-1.8049E-03	5.0889E-03	6.8938E-03
14.00	-1.4291E-03	4.2910E-03	5.7201E-03
14.50	-1.1788E-03	3.7908E-03	4.9696E-03
15.00	-1.0313E-03	3.5027E-03	4.5340E-03
15.50	-9.3047E-04	3.0079E-03	3.9384E-03
16.00	-8.3139E-04	2.4244E-03	3.2558E-03
16.50	-7.1536E-04	2.1511E-03	2.8665E-03
17.00	-5.8516E-04	1.9110E-03	2.4962E-03
17.50	-4.5343E-04	1.7891E-03	2.2425E-03
18.00	-3.3308E-04	1.7383E-03	2.0714E-03
18.50	-2.3242E-04	1.7365E-03	1.9689E-03
19.00	-1.5437E-04	1.6072E-03	1.7616E-03
19.50	-9.7694E-05	1.2757E-03	1.3734E-03
20.00	-5.8898E-05	1.3136E-03	1.3725E-03
20.50	-3.3763E-05	1.2959E-03	1.3297E-03
21.00	-1.8330E-05	1.2213E-03	1.2396E-03
21.50	-9.3594E-06	1.1988E-03	1.2082E-03
22.00	-4.4479E-06	1.2245E-03	1.2289E-03

Table S13

Triplet R (a.u.)	Total Hexadecapole Φ_{zzzz}		
	daug6Z HF Φ_{zzzz} Tot	daug6Z FCI Φ_{zzzz} Tot	daug6Z Correlation
5.00	-1.1696E+00	-1.1043E+00	6.5300E-02
5.50	-8.1942E-01	-7.4346E-01	7.5960E-02
6.00	-5.4521E-01	-4.6642E-01	7.8790E-02
6.50	-3.4648E-01	-2.7081E-01	7.5670E-02
7.00	-2.1098E-01	-1.4204E-01	6.8940E-02
7.50	-1.2311E-01	-6.2611E-02	6.0499E-02
7.85	-8.2129E-02	-2.7819E-02	5.4310E-02
8.00	-6.8497E-02	-1.7071E-02	5.1426E-02
8.50	-3.5790E-02	7.3891E-03	4.3179E-02
9.00	-1.6833E-02	1.8985E-02	3.5818E-02
9.50	-6.0564E-03	2.3593E-02	2.9649E-02
10.00	1.5351E-04	2.4670E-02	2.4516E-02
10.50	3.7665E-03	2.4099E-02	2.0333E-02
11.00	5.5888E-03	2.2534E-02	1.6945E-02
11.50	6.0708E-03	2.0249E-02	1.4178E-02
12.00	5.8462E-03	1.7499E-02	1.1653E-02
12.50	5.6341E-03	1.5361E-02	9.7269E-03
13.00	5.8567E-03	1.4163E-02	8.3063E-03
13.50	6.4765E-03	1.3656E-02	7.1795E-03
14.00	7.1603E-03	1.3295E-02	6.1347E-03
14.50	7.5510E-03	1.2817E-02	5.2660E-03
15.00	7.4462E-03	1.1962E-02	4.5158E-03
15.50	6.8300E-03	1.0883E-02	4.0530E-03
16.00	5.8174E-03	9.3619E-03	3.5445E-03
16.50	4.5780E-03	7.7082E-03	3.1302E-03
17.00	3.2784E-03	6.0010E-03	2.7226E-03
17.50	2.0512E-03	4.4791E-03	2.4279E-03
18.00	9.8453E-04	3.1089E-03	2.1244E-03
18.50	1.2366E-04	2.0034E-03	1.8797E-03
19.00	-5.2132E-04	1.1659E-03	1.6872E-03
19.50	-9.6552E-04	6.4516E-04	1.6107E-03
20.00	-1.2393E-03	3.0145E-04	1.5408E-03
20.50	-1.3795E-03	1.5116E-04	1.5307E-03
21.00	-1.4231E-03	-9.9812E-05	1.3233E-03
21.50	-1.4029E-03	-2.9549E-04	1.1074E-03
22.00	-1.3453E-03	-4.7553E-04	8.6977E-04

Table S14

Dispersion dipole μ_z in a.u. obtained with various basis sets

R (a.u)	pV6Z	augpV5Z	augpV6Z	daugpV5Z	daugpV6Z
12.0	-3.7226E-06	-1.1175E-05	-1.2186E-05	-1.3894E-05	-1.3632E-05
12.5	-2.7613E-06	-8.3596E-06	-8.9251E-06	-1.0148E-05	-1.0002E-05
13.0	-2.0790E-06	-6.2704E-06	-6.6784E-06	-7.6015E-06	-7.4835E-06
13.5	-1.5669E-06	-4.7769E-06	-5.0795E-06	-5.7537E-06	-5.6800E-06
14.0	-1.1909E-06	-3.6697E-06	-3.8971E-06	-4.3972E-06	-4.3886E-06
14.5	-7.8425E-07	-2.8450E-06	-3.0259E-06	-3.3883E-06	-3.3252E-06
15.0	-6.0184E-07	-2.1480E-06	-2.3722E-06	-2.7134E-06	-2.5710E-06
15.5	-4.7584E-07	-1.6771E-06	-1.8636E-06	-2.1623E-06	-2.0450E-06
16.0	-3.9555E-07	-1.3563E-06	-1.4315E-06	-1.6922E-06	-1.6275E-06
16.5	-3.1640E-07	-1.0805E-06	-1.1350E-06	-1.2953E-06	-1.2944E-06
17.0	-2.5650E-07	-8.7379E-07	-9.1871E-07	-1.0625E-06	-1.0332E-06
17.5	-2.0625E-07	-6.3482E-07	-7.4764E-07	-8.4519E-07	-8.3643E-07
18.0	-1.7377E-07	-5.9356E-07	-5.8662E-07	-6.8475E-07	-6.5698E-07
18.5	-1.3946E-07	-5.1206E-07	-5.1865E-07	-5.7600E-07	-5.4327E-07
19.0	-1.1727E-07	-4.2967E-07	-3.9670E-07	-4.7046E-07	-4.4296E-07
19.5	-9.7850E-08	-3.7573E-07	-3.4961E-07	-3.5936E-07	-3.6654E-07
20.0	-8.0532E-08	-3.2588E-07	-2.9031E-07	-2.6001E-07	-3.3380E-07
20.5	-6.7918E-08	-2.5078E-07	-2.4846E-07	-2.1638E-07	-2.8610E-07
21.0	-5.6873E-08	-1.7100E-07	-2.1160E-07	-1.8122E-07	-2.3471E-07
21.5	-4.7541E-08	-1.4366E-07	-1.8807E-07	-1.5175E-07	-1.8649E-07
22.0	-4.1196E-08	-1.2278E-07	-1.7043E-07	-1.2822E-07	-1.4673E-07

Table S15

Triplet R (a.u.)	Dispersion Charges		
	One center	Overlap	Total
5.0	-3.59356E-04	3.59376E-04	4.03074E-08
5.1	-3.54901E-04	3.54882E-04	-3.73507E-08
5.2	-3.47614E-04	3.47696E-04	1.62709E-07
5.3	-3.37684E-04	3.37767E-04	1.66192E-07
5.4	-3.25814E-04	3.25791E-04	-4.58514E-08
5.5	-3.12342E-04	3.12356E-04	2.86797E-08
5.6	-2.97652E-04	2.97625E-04	-5.44614E-08
5.7	-2.81946E-04	2.81979E-04	6.56369E-08
5.8	-2.65766E-04	2.65725E-04	-8.10766E-08
5.9	-2.49231E-04	2.49161E-04	-1.41130E-07
6.0	-2.32668E-04	2.32599E-04	-1.37947E-07
6.1	-2.16005E-04	2.16057E-04	1.04010E-07
6.2	-1.99831E-04	1.99800E-04	-6.17946E-08
6.3	-1.84172E-04	1.84086E-04	-1.72184E-07
6.4	-1.69004E-04	1.68924E-04	-1.59670E-07
6.5	-1.54539E-04	1.54418E-04	-2.42074E-07
6.6	-1.40837E-04	1.40752E-04	-1.71248E-07
6.7	-1.27847E-04	1.27848E-04	2.06514E-09
6.8	-1.15753E-04	1.15774E-04	4.16048E-08
6.9	-1.04564E-04	1.04544E-04	-3.90567E-08
7.0	-9.41094E-05	9.41953E-05	1.71737E-07
7.1	-8.46623E-05	8.46722E-05	1.98685E-08
7.2	-7.59404E-05	7.59247E-05	-3.14017E-08
7.3	-6.78194E-05	6.79272E-05	2.15595E-07
7.4	-6.06895E-05	6.06737E-05	-3.17509E-08
7.5	-5.41090E-05	5.40983E-05	-2.14392E-08
7.6	-4.80390E-05	4.81224E-05	1.66749E-07
7.7	-4.27040E-05	4.27633E-05	1.18618E-07
7.8	-3.79276E-05	3.79531E-05	5.10504E-08
7.9	-3.36109E-05	3.36191E-05	1.64680E-08
8.0	-2.96391E-05	2.97390E-05	1.99785E-07
8.1	-2.61530E-05	2.62517E-05	1.97530E-07
8.2	-2.31598E-05	2.31750E-05	3.03199E-08
8.3	-2.03595E-05	2.04330E-05	8.77313E-08
8.4	-1.79395E-05	1.79396E-05	2.39620E-10
8.5	-1.58337E-05	1.57824E-05	-1.02536E-07
8.6	-1.38290E-05	1.38351E-05	1.20408E-08
8.7	-1.21110E-05	1.21435E-05	6.49566E-08
8.8	-1.07096E-05	1.06426E-05	-1.33986E-07
8.9	-9.30725E-06	9.29997E-06	-1.45507E-08

9.0	-8.10474E-06	8.11190E-06	1.43200E-08
9.1	-7.06600E-06	7.08529E-06	3.85677E-08
9.2	-6.19621E-06	6.17868E-06	-3.50531E-08
9.3	-5.44099E-06	5.38040E-06	-1.21177E-07
9.4	-4.72981E-06	4.67937E-06	-1.00875E-07
9.5	-4.09302E-06	4.07410E-06	-3.78232E-08
9.6	-3.59562E-06	3.53554E-06	-1.20165E-07
9.7	-3.09897E-06	3.07262E-06	-5.27025E-08
9.8	-2.71453E-06	2.66448E-06	-1.00099E-07
9.9	-2.31836E-06	2.30468E-06	-2.73569E-08
10.0	-1.97999E-06	2.00371E-06	4.74256E-08

Table S16	CAS(2,2)	H2 singlet	d-aug-cc-pV6Z		
R	E CAS(2,2)	E FCI	Disp E	CAS DMA dipole	CAS DMA quad
12.0	-0.99999858	-1.00000110	-0.00000252	-5.8794E-07	1.9730E-05
12.5	-0.99999857	-1.00000052	-0.00000195	-6.3313E-07	1.1175E-05
13.0	-0.99999857	-1.00000009	-0.00000152	-6.8468E-07	6.8473E-06
13.5	-0.99999856	-0.99999977	-0.00000121	-7.3734E-07	5.2768E-06
14.0	-0.99999856	-0.99999952	-0.00000096	-7.7137E-07	4.9585E-06
14.5	-0.99999856	-0.99999933	-0.00000077	-7.6328E-07	4.8914E-06
15.0	-0.99999856	-0.99999919	-0.00000063	-7.0416E-07	4.6224E-06
15.5	-0.99999856	-0.99999907	-0.00000051	-6.0196E-07	4.0717E-06
16.0	-0.99999856	-0.99999898	-0.00000042	-4.7417E-07	3.3352E-06
16.5	-0.99999856	-0.99999891	-0.00000035	-3.3969E-07	2.5477E-06
17.0	-0.99999856	-0.99999885	-0.00000029	-2.1375E-07	1.8164E-06
17.5	-0.99999856	-0.99999880	-0.00000024	-1.0613E-07	1.2035E-06
18.0	-0.99999856	-0.99999876	-0.00000020	-2.1290E-08	7.3121E-07
18.5	-0.99999856	-0.99999873	-0.00000017	4.0378E-08	3.9492E-07
19.0	-0.99999856	-0.99999871	-0.00000015	8.1219E-08	1.7509E-07
19.5	-0.99999856	-0.99999868	-0.00000012	1.0497E-07	4.6375E-08
20.0	-0.99999856	-0.99999867	-0.00000011	1.1580E-07	-1.6537E-08
20.5	-0.99999856	-0.99999865	-0.00000009	1.1760E-07	-3.5776E-08
21.0	-0.99999856	-0.99999864	-0.00000008	1.1367E-07	-2.8890E-08
21.5	-0.99999856	-0.99999863	-0.00000007	1.0651E-07	-8.6334E-09
22.0	-0.99999856	-0.99999862	-0.00000006	9.7909E-08	1.6403E-08
R	E CAS(2,2)	E FCI	Disp E	CAS DMA octo	CAS DMA hexa
12.0	-0.99999858	-1.00000110	-0.00000252	1.0447E-04	1.1186E-03
12.5	-0.99999857	-1.00000052	-0.00000195	2.2586E-05	3.6381E-04
13.0	-0.99999857	-1.00000009	-0.00000152	-2.5563E-05	-1.2002E-04
13.5	-0.99999856	-0.99999977	-0.00000121	-4.8508E-05	-3.7154E-04
14.0	-0.99999856	-0.99999952	-0.00000096	-5.5233E-05	-4.5826E-04
14.5	-0.99999856	-0.99999933	-0.00000077	-5.2702E-05	-4.4606E-04
15.0	-0.99999856	-0.99999919	-0.00000063	-4.5594E-05	-3.8513E-04
15.5	-0.99999856	-0.99999907	-0.00000051	-3.6773E-05	-3.0741E-04
16.0	-0.99999856	-0.99999898	-0.00000042	-2.7865E-05	-2.3024E-04
16.5	-0.99999856	-0.99999891	-0.00000035	-1.9723E-05	-1.6153E-04
17.0	-0.99999856	-0.99999885	-0.00000029	-1.2754E-05	-1.0407E-04
17.5	-0.99999856	-0.99999880	-0.00000024	-7.1014E-06	-5.8155E-05
18.0	-0.99999856	-0.99999876	-0.00000020	-2.7484E-06	-2.2986E-05
18.5	-0.99999856	-0.99999873	-0.00000017	4.2103E-07	2.7589E-06
19.0	-0.99999856	-0.99999871	-0.00000015	2.5825E-06	2.0630E-05
19.5	-0.99999856	-0.99999868	-0.00000012	3.9382E-06	3.2245E-05
20.0	-0.99999856	-0.99999867	-0.00000011	4.6892E-06	3.9157E-05
20.5	-0.99999856	-0.99999865	-0.00000009	5.0165E-06	4.2745E-05
21.0	-0.99999856	-0.99999864	-0.00000008	5.0692E-06	4.4151E-05
21.5	-0.99999856	-0.99999863	-0.00000007	4.9609E-06	4.4257E-05
22.0	-0.99999856	-0.99999862	-0.00000006	4.7716E-06	4.3689E-05

CAS total quad	FCI DMA dipole	FCI DMA quad	FCI total quad	Disp DMA dipole	Disp DMA quad	Disp total quad
5.3570E-05	-1.4362E-05	-1.5804E-05	3.1308E-04	-1.3774E-05	-3.5534E-05	2.5951E-04
3.8179E-05	-1.0859E-05	-1.4872E-05	2.4172E-04	-1.0226E-05	-2.6047E-05	2.0354E-04
3.1496E-05	-8.2694E-06	-1.2625E-05	1.8975E-04	-7.5847E-06	-1.9472E-05	1.5825E-04
3.0462E-05	-6.2416E-06	-9.4346E-06	1.4965E-04	-5.5043E-06	-1.4711E-05	1.1919E-04
3.1515E-05	-5.0570E-06	-6.3898E-06	1.2882E-04	-4.2856E-06	-1.1348E-05	9.7305E-05
3.1918E-05	-4.0428E-06	-4.0279E-06	1.0919E-04	-3.2795E-06	-8.9193E-06	7.7272E-05
3.0369E-05	-3.3034E-06	-2.4558E-06	9.4190E-05	-2.5992E-06	-7.0782E-06	6.3821E-05
2.6804E-05	-2.6212E-06	-1.6190E-06	7.8020E-05	-2.0192E-06	-5.6907E-06	5.1216E-05
2.1844E-05	-2.0682E-06	-1.2377E-06	6.3707E-05	-1.5940E-06	-4.5729E-06	4.1863E-05
1.6305E-05	-1.6128E-06	-1.1398E-06	5.0943E-05	-1.2731E-06	-3.6875E-06	3.4638E-05
1.0900E-05	-1.2411E-06	-1.1949E-06	3.9808E-05	-1.0274E-06	-3.0113E-06	2.8908E-05
6.1214E-06	-9.4185E-07	-1.2773E-06	3.0410E-05	-8.3572E-07	-2.4808E-06	2.4289E-05
2.2289E-06	-7.0539E-07	-1.3325E-06	2.2729E-05	-6.8410E-07	-2.0637E-06	2.0500E-05
-7.0422E-07	-5.1571E-07	-1.3187E-06	1.6444E-05	-5.5609E-07	-1.7136E-06	1.7148E-05
-2.7361E-06	-3.6748E-07	-1.2607E-06	1.1443E-05	-4.4870E-07	-1.4358E-06	1.4179E-05
-4.0011E-06	-2.8225E-07	-1.1769E-06	8.6540E-06	-3.8722E-07	-1.2233E-06	1.2655E-05
-4.6650E-06	-2.0401E-07	-1.0159E-06	6.1286E-06	-3.1981E-07	-9.9936E-07	1.0794E-05
-4.8933E-06	-1.5020E-07	-8.9188E-07	4.3743E-06	-2.6780E-07	-8.5610E-07	9.2676E-06
-4.8319E-06	-1.0639E-07	-7.7977E-07	2.9088E-06	-2.2006E-07	-7.5088E-07	7.7407E-06
-4.5973E-06	-4.9381E-08	-6.0890E-07	9.0563E-07	-1.5589E-07	-6.0027E-07	5.5029E-06
-4.2752E-06	-3.5378E-08	-5.0172E-07	5.5322E-07	-1.3329E-07	-5.1812E-07	4.8284E-06
CAS total hexa	FCI DMA octo	FCI DMA hexa	FCI total hexa	Disp DMA octo	Disp DMA hexa	Disp total hexa
6.7618E-03	3.2476E-05	9.0654E-04	1.8245E-02	-7.1994E-05	-2.1206E-04	1.1483E-02
6.0734E-03	-2.6255E-05	2.3298E-04	1.6015E-02	-4.8841E-05	-1.3083E-04	9.9416E-03
6.0651E-03	-5.9460E-05	-2.0119E-04	1.4456E-02	-3.3897E-05	-8.1170E-05	8.3909E-03
6.5756E-03	-7.2941E-05	-4.2526E-04	1.3287E-02	-2.4433E-05	-5.3720E-05	6.7114E-03
7.2088E-03	-7.2756E-05	-4.9112E-04	1.3211E-02	-1.7523E-05	-3.2860E-05	6.0022E-03
7.5768E-03	-6.5639E-05	-4.6810E-04	1.2655E-02	-1.2937E-05	-2.2040E-05	5.0782E-03
7.4620E-03	-5.5148E-05	-3.9986E-04	1.2000E-02	-9.5540E-06	-1.4730E-05	4.5380E-03
6.8414E-03	-4.4193E-05	-3.1757E-04	1.0699E-02	-7.4200E-06	-1.0160E-05	3.8576E-03
5.8265E-03	-3.3721E-05	-2.3714E-04	9.2047E-03	-5.8560E-06	-6.9000E-06	3.3782E-03
4.5854E-03	-2.4061E-05	-1.6653E-04	7.5689E-03	-4.3380E-06	-5.0000E-06	2.9835E-03
3.2842E-03	-1.6178E-05	-1.0768E-04	5.9463E-03	-3.4240E-06	-3.6100E-06	2.6621E-03
2.0553E-03	-9.8375E-06	-6.1183E-05	4.4405E-03	-2.7361E-06	-3.0280E-06	2.3852E-03
9.8682E-04	-5.0019E-06	-2.5067E-05	3.1286E-03	-2.2535E-06	-2.0810E-06	2.1418E-03
1.2417E-04	-1.4113E-06	9.1350E-07	2.0176E-03	-1.8323E-06	-1.8454E-06	1.8934E-03
-5.2247E-04	1.0535E-06	1.9393E-05	1.1140E-03	-1.5290E-06	-1.2370E-06	1.6365E-03
-9.6812E-04	2.6752E-06	3.1257E-05	6.0415E-04	-1.2630E-06	-9.8800E-07	1.5723E-03
-1.2430E-03	3.6468E-06	3.8231E-05	1.9774E-04	-1.0424E-06	-9.2600E-07	1.4407E-03
-1.3842E-03	4.1512E-06	4.1990E-05	-8.6899E-05	-8.6530E-07	-7.5500E-07	1.2973E-03
-1.4284E-03	4.3485E-06	4.3530E-05	-3.2458E-04	-7.2070E-07	-6.2100E-07	1.1038E-03
-1.4087E-03	4.8041E-06	4.4090E-05	-6.7859E-04	-1.5680E-07	-1.6700E-07	7.3011E-04
-1.3512E-03	4.6364E-06	4.3543E-05	-6.7269E-04	-1.3520E-07	-1.4600E-07	6.7851E-04

Table S17

He-H aug-cc-pV5Z

R	RHF dipole on H	FCI dipole on H	RHF dipole on He	FCI dipole on He	Corr dipole on H	Corr dipole on He
10	1.9521E-06	-1.5680E-05	2.2682E-06	6.9017E-06	-1.7632E-05	4.6335E-06
11	3.0883E-07	-8.2877E-06	2.0283E-06	4.1966E-06	-8.5965E-06	2.1683E-06
12	-4.5531E-07	-4.9458E-06	9.4781E-07	2.0854E-06	-4.4905E-06	1.1376E-06
13	-3.5346E-07	-2.6898E-06	4.4695E-07	1.2774E-06	-2.3363E-06	8.3045E-07
14	-1.5215E-07	-1.5503E-06	2.2218E-07	7.4079E-07	-1.3982E-06	5.1861E-07
15	-4.3890E-08	-8.5242E-07	1.0281E-07	4.6362E-07	-8.0853E-07	3.6081E-07
16	-6.4347E-09	-5.2185E-07	4.2032E-08	2.4813E-07	-5.1542E-07	2.0610E-07
17	1.3670E-09	-3.4544E-07	1.5122E-08	1.3876E-07	-3.4681E-07	1.2364E-07
18	1.3596E-09	-1.9290E-07	4.7821E-09	8.1326E-08	-1.9426E-07	7.6544E-08
19	5.6791E-10	-1.0697E-07	1.3054E-09	5.2603E-08	-1.0754E-07	5.1298E-08
20	1.7137E-10	-8.0367E-08	2.8982E-10	3.3090E-08	-8.0538E-08	3.2800E-08

R	RHF total dipole	FCI total dipole	Dispersion dipole
10	3.8190E-06	-9.9859E-06	-1.3805E-05
11	-9.1970E-08	-6.7486E-06	-6.6566E-06
12	-5.3795E-07	-3.9828E-06	-3.4449E-06
13	-2.2841E-07	-1.7664E-06	-1.5380E-06
14	-2.3992E-08	-9.1145E-07	-8.8746E-07
15	3.7492E-08	-4.1077E-07	-4.4826E-07
16	3.5419E-08	-2.7307E-07	-3.0849E-07
17	1.9867E-08	-2.0258E-07	-2.2245E-07
18	8.5342E-09	-1.0875E-07	-1.1728E-07
19	3.0333E-09	-5.2992E-08	-5.6025E-08
20	9.2503E-10	-4.6714E-08	-4.7639E-08

He-H aug-cc-pV6Z

R	RHF dipole on H	FCI dipole on H	RHF dipole on He	FCI dipole on He	Corr dipole on H	Corr dipole on He
10	-2.2372E-08	-1.8713E-05	-1.0609E-06	3.9771E-06	-1.8691E-05	5.0380E-06
11	3.4774E-07	-8.9596E-06	5.6617E-07	2.9256E-06	-9.3073E-06	2.3594E-06
12	6.7961E-08	-4.8227E-06	4.4896E-07	1.6561E-06	-4.8907E-06	1.2071E-06
13	-9.4046E-08	-2.7835E-06	2.1366E-07	8.9293E-07	-2.6895E-06	6.7927E-07
14	-8.4809E-08	-1.5613E-06	1.1068E-07	6.1767E-07	-1.4765E-06	5.0699E-07
15	-4.3343E-08	-8.7781E-07	6.3989E-08	3.9737E-07	-8.3447E-07	3.3338E-07
16	-1.5866E-08	-5.5873E-07	3.4893E-08	2.6423E-07	-5.4286E-07	2.2934E-07
17	-3.9968E-09	-3.3693E-07	1.6912E-08	1.6195E-07	-3.3293E-07	1.4504E-07
18	-4.6609E-10	-2.3237E-07	7.3344E-09	1.0431E-07	-2.3190E-07	9.6976E-08
19	1.4099E-10	-1.6143E-07	2.8930E-09	6.9249E-08	-1.6157E-07	6.6356E-08
20	1.0877E-10	-1.0826E-07	1.0498E-09	4.3163E-08	-1.0837E-07	4.2113E-08

R	RHF total dipole	FCI total dipole	Dispersion dipole
---	------------------	------------------	-------------------

10	3.3429E-06	-1.1422E-05	-1.4765E-05
11	8.9099E-07	-6.2463E-06	-7.1373E-06
12	1.1267E-07	-3.6125E-06	-3.7252E-06
13	-3.9449E-08	-2.0680E-06	-2.0286E-06
14	-1.1620E-08	-9.9053E-07	-9.7891E-07
15	1.5077E-08	-4.9038E-07	-5.0546E-07
16	2.0404E-08	-2.9499E-07	-3.1539E-07
17	1.5241E-08	-1.7342E-07	-1.8866E-07
18	8.5611E-09	-1.2668E-07	-1.3524E-07
19	3.9519E-09	-9.1380E-08	-9.5332E-08
20	1.5712E-09	-6.4730E-08	-6.6301E-08

He-H d-aug-cc-pV5Z

R	RHF dipole on H	FCI dipole on H	RHF dipole on He	FCI dipole on He	Corr dipole on H	Corr dipole on He
---	-----------------	-----------------	------------------	------------------	------------------	-------------------

10	-3.6678E-05	-5.9136E-05	-3.5577E-05	-3.0946E-05	-2.2458E-05	4.6310E-06
11	-8.9411E-06	-1.9772E-05	-2.4806E-06	-4.7302E-07	-1.0831E-05	2.0076E-06
12	-9.3648E-07	-6.3808E-06	2.8142E-06	3.6919E-06	-5.4443E-06	8.7770E-07
13	3.0224E-08	-2.8663E-06	1.0145E-06	1.3913E-06	-2.8965E-06	3.7680E-07
14	2.5314E-07	-1.4066E-06	-3.9060E-07	-1.5695E-07	-1.6597E-06	2.3365E-07
15	4.1917E-07	-4.0140E-07	-8.1188E-07	-7.9070E-07	-8.2057E-07	2.1180E-08
16	4.1805E-07	-5.1662E-08	-8.0734E-07	-4.6035E-07	-4.6971E-07	3.4699E-07
17	3.1640E-07	5.5136E-08	-6.9575E-07	-2.1128E-07	-2.6126E-07	4.8447E-07
18	2.0242E-07	6.1992E-08	-5.8058E-07	-1.5472E-07	-1.4043E-07	4.2586E-07
19	1.1385E-07	5.7343E-08	-4.8290E-07	-1.8330E-07	-5.6507E-08	2.9960E-07
20	5.5432E-08	3.3024E-08	-4.0097E-07	-2.2808E-07	-2.2408E-08	1.7289E-07

R	RHF total dipole	FCI total dipole	Dispersion dipole
---	------------------	------------------	-------------------

10	2.9898E-06	-1.4094E-05	-1.7084E-05
11	2.5225E-06	-5.8732E-06	-8.3957E-06
12	-7.1842E-08	-4.5846E-06	-4.5128E-06
13	-1.6215E-06	-4.1919E-06	-2.5704E-06
14	-1.6352E-06	-3.0985E-06	-1.4633E-06
15	-1.1909E-06	-1.9945E-06	-8.0360E-07
16	-7.9602E-07	-9.0748E-07	-1.1146E-07
17	-5.1905E-07	-2.8100E-07	2.3805E-07
18	-3.3226E-07	-3.4189E-08	2.9807E-07
19	-2.0942E-07	4.2672E-08	2.5209E-07
20	-1.3175E-07	2.4640E-08	1.5639E-07

He-H d-aug-cc-pV6Z

R	RHF dipole on H	FCI dipole on H	RHF dipole on He	FCI dipole on He	Corr dipole on H	Corr dipole on He
10	-1.3144E-05	-3.4332E-05	-1.6365E-05	-1.1028E-05	-2.1188E-05	5.3370E-06
11	-7.1252E-06	-1.7559E-05	-5.8451E-06	-3.7017E-06	-1.0434E-05	2.1434E-06
12	-1.9350E-06	-7.3187E-06	-4.6008E-07	3.7090E-07	-5.3837E-06	8.3098E-07
13	-3.4665E-07	-3.3021E-06	5.2363E-07	8.5023E-07	-2.9555E-06	3.2660E-07
14	-1.4665E-07	-1.8094E-06	1.4890E-07	2.7307E-07	-1.6628E-06	1.2417E-07
15	-4.1818E-08	-1.0278E-06	-1.8417E-07	-2.2728E-08	-9.8598E-07	1.6144E-07
16	7.8500E-08	-5.1487E-07	-2.8333E-07	4.6812E-09	-5.9337E-07	2.8801E-07
17	1.3358E-07	-2.3366E-07	-2.6392E-07	-2.9411E-08	-3.6724E-07	2.3451E-07
18	1.2795E-07	-9.9798E-08	-2.1580E-07	-4.7719E-08	-2.2775E-07	1.6808E-07
19	9.7553E-08	-5.0057E-08	-1.7236E-07	-4.7172E-08	-1.4761E-07	1.2519E-07
20	6.5729E-08	-4.2424E-08	-1.3913E-07	-5.0887E-08	-1.0815E-07	8.8243E-08

R	RHF total dipole	FCI total dipole	Dispersion dipole
10	2.0011E-06	-1.5496E-05	-1.7497E-05
11	5.4961E-07	-8.0662E-06	-8.6158E-06
12	3.6602E-07	-4.2595E-06	-4.6255E-06
13	-2.9929E-07	-2.9469E-06	-2.6476E-06
14	6.9017E-07	-2.2274E-06	-2.9176E-06
15	-6.4209E-07	-1.4559E-06	-8.1381E-07
16	-4.4056E-07	-7.3273E-07	-2.9217E-07
17	-2.6603E-07	-3.8711E-07	-1.2108E-07
18	-1.5260E-07	-2.0372E-07	-5.1120E-08
19	-8.5688E-08	-1.0269E-07	-1.7002E-08
20	-4.8302E-08	-6.5266E-08	-1.6964E-08

Table S18

He-He	d-aug-cc-pV5Z		
R (a.u.)	RHF DMA dipole	FCI DMA dipole	Dispersion DMA dipole
8	8.0169E-06	-4.2762E-06	-1.2293E-05
9	-6.0562E-06	-1.1471E-05	-5.4148E-06
10	-3.4414E-06	-5.8567E-06	-2.4153E-06
11	-6.5195E-07	-1.7945E-06	-1.1426E-06
12	7.2295E-07	1.9528E-07	-5.2767E-07
13	1.0588E-06	7.3811E-07	-3.2069E-07
14	9.7153E-07	7.3857E-07	-2.3296E-07
15	7.8241E-07	6.2786E-07	-1.5455E-07
16	5.9927E-07	4.8482E-07	-1.1445E-07
17	4.4559E-07	3.6532E-07	-8.0270E-08
18	3.2192E-07	2.6462E-07	-5.7300E-08
19	2.2513E-07	1.8345E-07	-4.1680E-08
20	1.5191E-07	1.2601E-07	-2.5900E-08

Table S19. Results from Eq. (16)¹³¹ for the number of Configuration State Functions (CSFs) and the number of determinants for the FCI functions in various basis sets

Number of configuration state functions at FCI level from the Weyl-Paldus formula

Basis set	Orbitals	CSFs for H-H	CSFs for H-He	CSFs for He-He
aug-cc-pV5Z	160	12,720	1,365,280	54,611,200
aug-cc-pV6Z	254	32,131	5,462,270	346,854,145
d-aug-cc-pV5Z	210	21,945	3,086,930	162,063,825
d-aug-cc-pV6Z	326	52,975	11,548,550	941,205,825
t-aug-cc-pV5Z	260	33,670	5,858,580	380,807,700

Number of determinants at FCI level, from Eq. (4.16) given by C. D. Sherrill, at <https://vergil.chemistry.gatech.edu/static/content/ci.pdf>

Basis set	Orbitals	Dets for H-H	Dets for H-He	Dets for He-He
aug-cc-pV5Z	160	12,720	2,035,200	161,798,400
aug-cc-pV6Z	254	32,131	8,161,274	1,032,401,161
d-aug-cc-pV5Z	210	21,945	4,608,450	481,583,025
d-aug-cc-pV6Z	326	52,975	17,269,850	2,806,350,625
t-aug-cc-pV5Z	260	33,670	8,754,200	1,133,668,900

Number of determinants at FCI level, taking symmetry into account

Basis set	Number of orbitals	Dets for He-He
aug-cc-pV5Z	160	20,357,888
aug-cc-pV6Z	254	129,502,585
d-aug-cc-pV5Z	210	60,531,525
d-aug-cc-pV6Z	326	350,793,828*
t-aug-cc-pV5Z	260	142,414,708

*Estimated number

Number of determinants of each symmetry in D_{2h}, He-He, d-aug-cc-pV5Z

Symmetry	Dets
Ag	60,531,525
B3u	60,197,500
B2u	60,197,500
B1g	59,870,500
B1u	60,520,500
B2g	60,197,500
B3g	60,197,500
Au	59,870,500

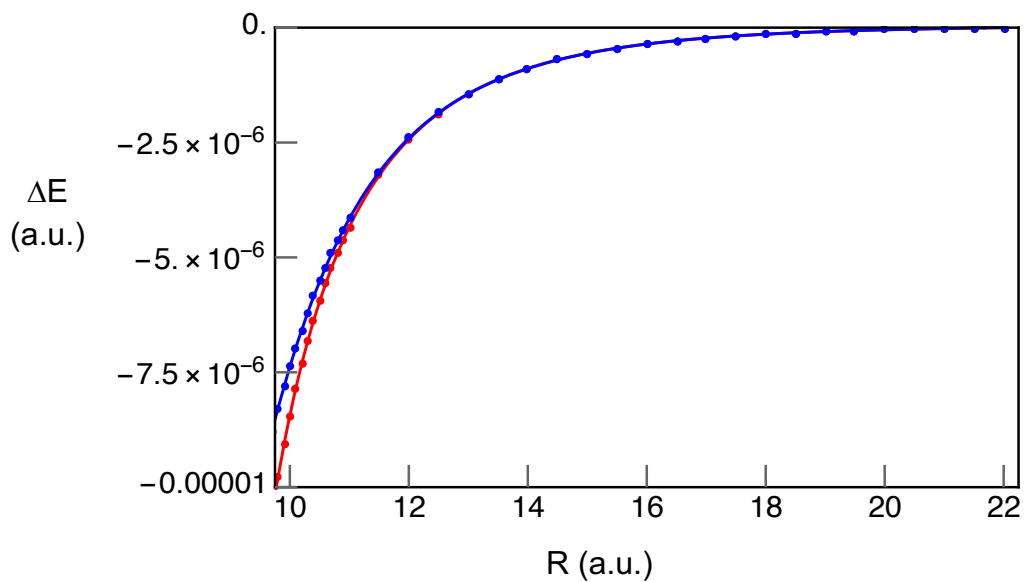


Figure S1. Long-range interaction energy in the triplet state (blue), and the singlet state (red), this work. The energies nearly coincide for $R > 12.0$ a.u.

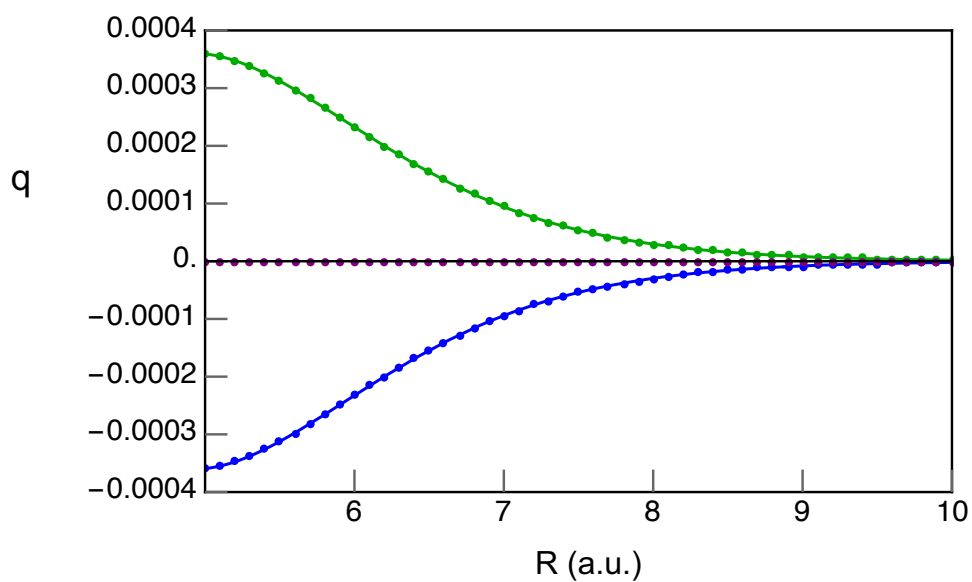


Figure S2. Green curve: Net dispersion charge q on the orbitals on a single center. Blue curve: One-half of the total overlap dispersion charge q , computed from dispersion density matrix elements with one orbital on one center and the other on the other center. Purple points: Total dispersion charge q ; the exact value would be zero.

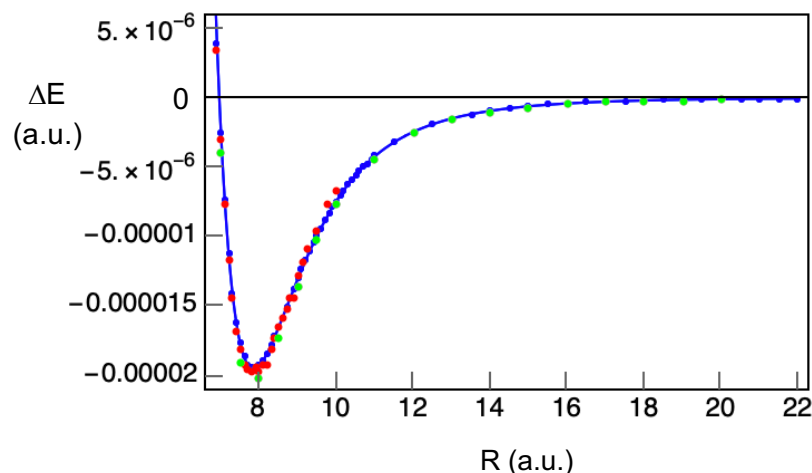


Figure S3. Blue points: Energies of the $b^3\Sigma_u^+$ state of H_2 obtained with the aug-cc-pV6Z basis. Blue curve: Mathematica interpolation of the triplet state energies. Red points: Energies obtained by W. Kołos and L. Wolniewicz, *J. Chem. Phys.* **43**, 2429 (1965). Green points: Energies obtained by Y. I. Kurokawa, H. Nakashima, and H. Nakatsuji, *Phys. Chem. Chem. Phys.* **21**, 6327 (2019); these points superimpose on the results obtained by G. Staszewska and L. Wolniewicz, *J. Mol. Spectrosc.* **198**, 416 (1999).

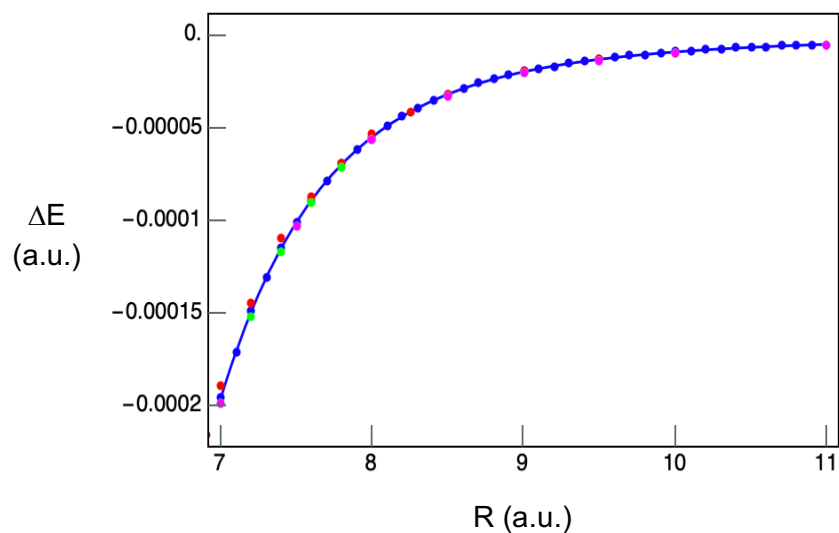


Figure S4. Blue points: Energies of the $X^1\Sigma_g^+$ state of H_2 obtained with the aug-cc-pV6Z basis. Blue curve: Mathematica interpolation of the singlet state energies. Red points: Energies obtained by W. Kołos and L. Wolniewicz, *J. Chem. Phys.* **43**, 2429 (1965). Green points: Energies obtained by W. Kołos and L. Wolniewicz, *J. Mol. Spectrosc.* **54**, 303 (1975). Cyan points: Y. I. Kurokawa, H. Nakashima, and H. Nakatsuji, *Phys. Chem. Chem. Phys.* **21**, 6327 (2019). Magenta points: K. Pachucki, *Phys. Rev. A* **82**, 032509 (2010).

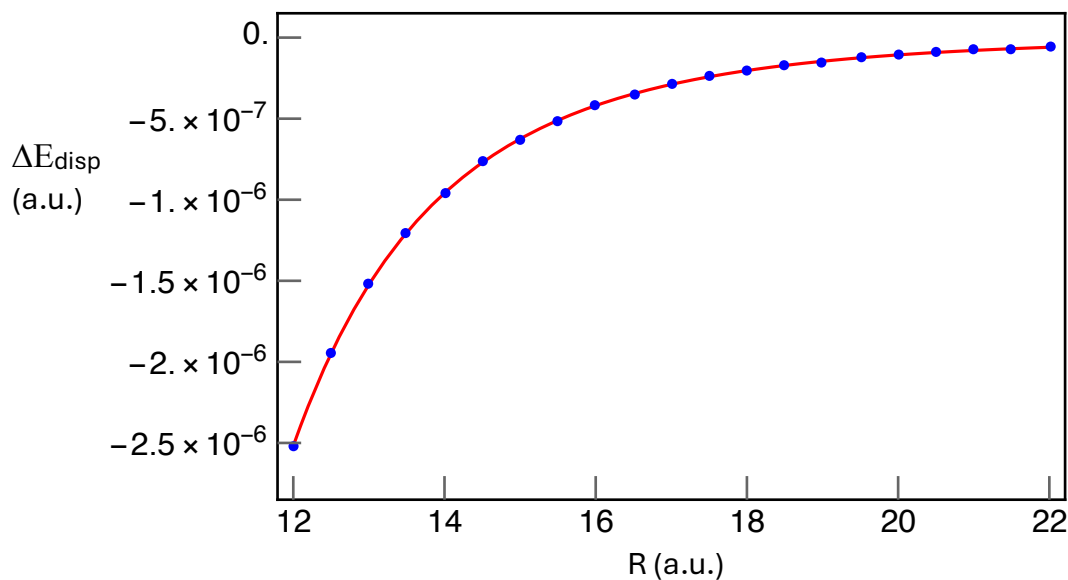


Figure S5. Dispersion energy of H_2 in the $X^1\Sigma_g^+$ state computed as the difference between the FCI energy and the CAS(2,2) energy in the d-aug-cc-pV6Z basis, compared with the long-range dispersion energy series including coefficients C_6 , C_8 , and C_{10} . The dispersion energy coefficients come from David M. Bishop and Janusz Pipin, Dipole, Quadrupole, Octupole, and Dipole-Octupole Polarizabilities at Real and Imaginary Frequencies of H, He, and H_2 and the Dispersion-Energy Coefficients for Interactions Between Them, *Int J. Quant Chem.* **45**, 349-361 (1993).

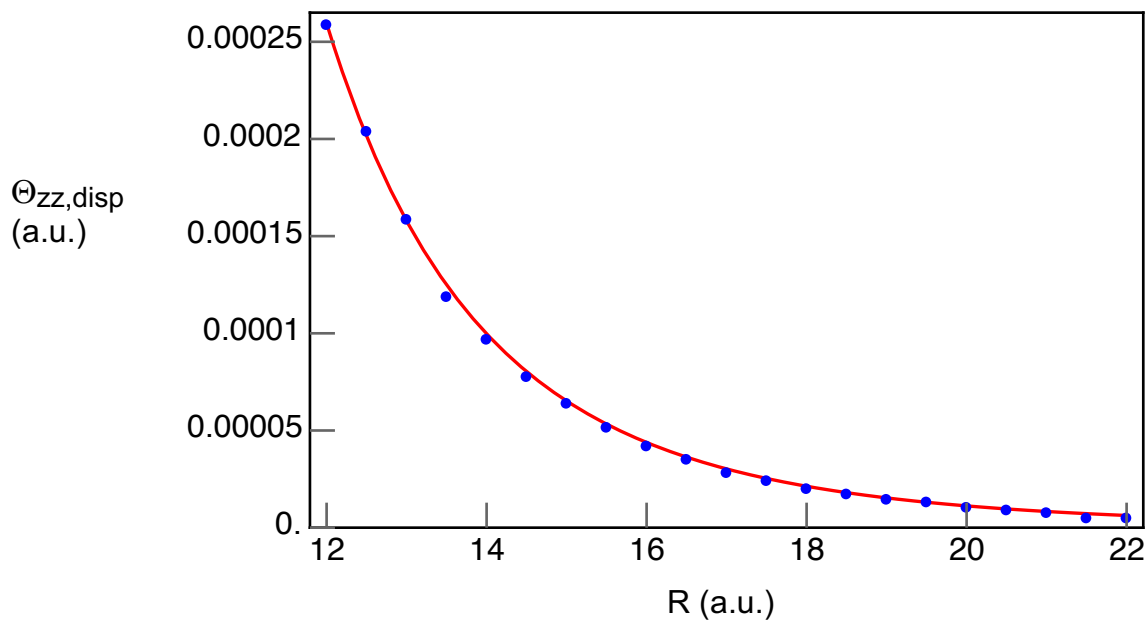


Figure S6. Total dispersion quadrupole of H_2 in the $X^1\Sigma_g^+$ state, compared with the long-range form from perturbation theory, with the same coefficients as found for the triplet state.

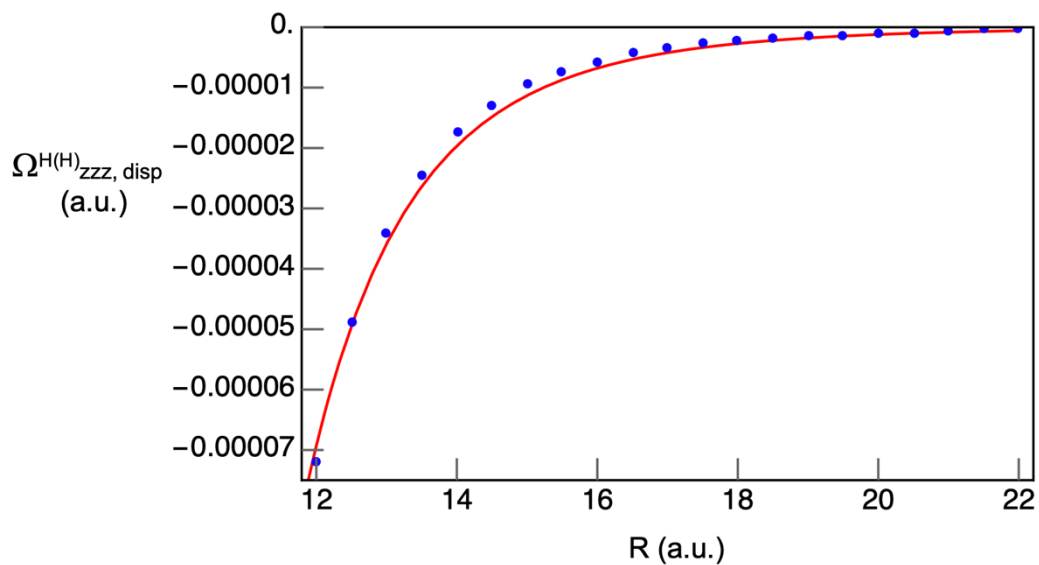


Figure S7. DMA dispersion octopole Ω_{zzz} on the H center at $(0, 0, -R/2)$ for the singlet state in the d-aug-cc-pV6Z basis.

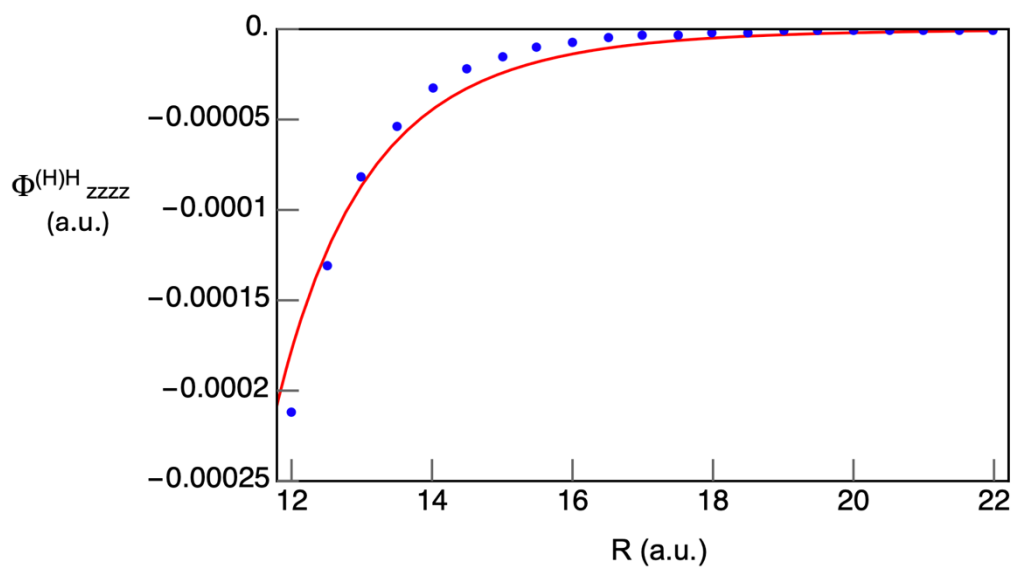


Figure S8. DMA dispersion hexadecapole Φ_{zzzz} on the H center at $(0, 0, -R/2)$ for the singlet state in the d-aug-cc-pV6Z basis.

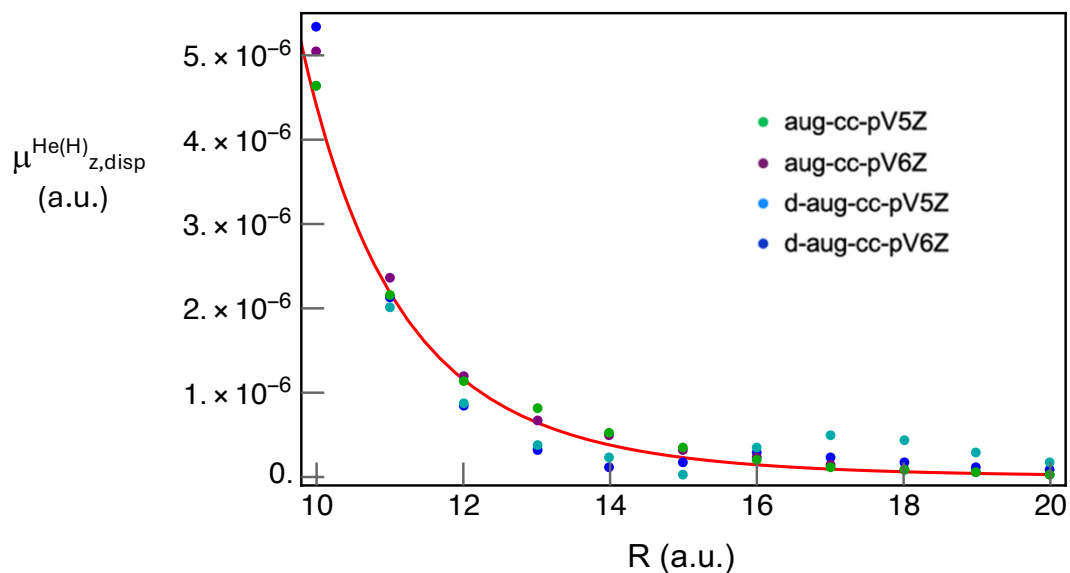


Figure S9. DMA dispersion dipole on the He center in HeH obtained with several different basis sets.

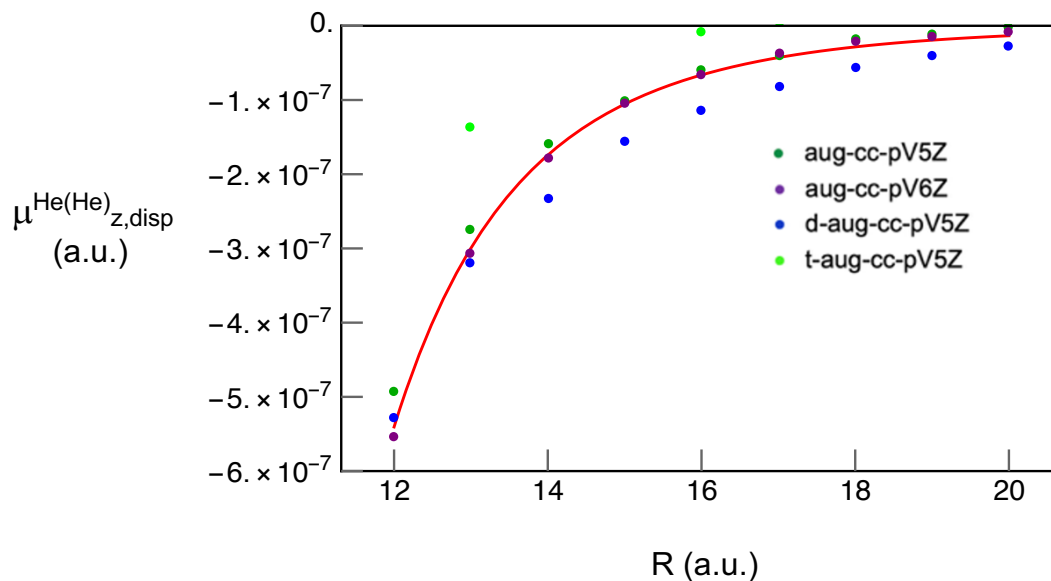


Figure S10. Close-up of the DMA dispersion dipole on the He center at (0, 0, -R/2) in He...He, in the range from R = 12 a.u. to 20 a.u., obtained with several different basis sets.