Nonadiabatic relativistic correction to the dissociation energy of H_2, HD, and D_2

Supplementary material for Physical Review Letters

In this supplement we present nonrelativistic energies and expectation values (in a.u.) of individual relativistic operators of Eq. (16) for different sizes of naECG basis sets, in order to demonstrate fast numerical convergence and for a possible comparison with any future calculations.

Basis	H_2	HD	D_2
		Nonrelativistic energy	
128	−1.164 023 669 155	−1.165 470 991 485	−1.167 167 911 358
256	−1.164 024 987 878	−1.165 471 628 967	−1.167 168 756 439
512	−1.164 025 027 334	−1.165 471 916 621	−1.167 168 805 491
1024	−1.164 025 030 593	−1.165 471 923 256	−1.167 168 808 953
2048	−1.164 025 030 843	−1.165 471 923 906	−1.167 168 809 193
naJC	−1.164 025 030 883 1(3)	−1.165 471 923 964 38(3)	−1.167 168 809 284 0(1)
		$Q_1 \equiv \left\langle p_2^4 + p_3^4 \right\rangle$	
128	13.006 596 49	13.039 285 64	13.076 429 013
256	13.007 278 21	13.039 464 31	13.076 715 179
512	13.007 296 39	13.039 557 52	13.076 753 607
1024	13.007 298 02	13.039 561 34	13.076 756 374
2048	13.007 297 58	13.039 561 74	13.076 756 860
∞	13.007 297 1(2)	13.039 561 82(11)	13.076 756 94(8)
		$Q_2 \equiv \left\langle \sum_{a,x} \left(1 + \frac{\delta_s}{m_x^2}\right) 4\pi\delta^3(r_{ax}) \right\rangle$	
128	11.346 037 956	11.374 443 161	11.407 118 222
256	11.346 455 251	11.374 536 486	11.407 269 494
512	11.346 474 224	11.374 592 915	11.407 288 516
1024	11.346 478 776	11.374 598 095	11.407 292 819
2048	11.346 479 559	11.374 598 758	11.407 293 510
∞	11.346 479 69(9)	11.374 598 84(8)	11.407 293 62(7)
		$Q_3 \equiv \left\langle 4\pi\delta^3(r) \right\rangle$	
128	0.202 801 005 5	0.203 819 224 9	0.204 997 246 3
256	0.202 827 947 7	0.203 830 085 0	0.205 010 952 8
512	0.202 829 969 6	0.203 833 611 3	0.205 012 853 1
1024	0.202 830 250 6	0.203 833 805 6	0.205 013 194 1
2048	0.202 830 297 3	0.203 833 855 6	0.205 013 230 5
∞	0.202 830 305(5)	0.203 833 868(9)	0.205 013 234(3)
		$Q_4 \cdot 10^2 \equiv \left\langle p_2^i \left(\frac{\delta^{ij}}{r} + \frac{r^i r^j}{r^3}\right) p_3^j \right\rangle \cdot 10^2$	
128	9.260 659 85	9.296 513 75	9.339 399 75
256	9.259 374 24	9.296 083 36	9.338 748 42
512	9.259 275 36	9.295 931 95	9.338 653 48
1024	9.259 263 40	9.295 923 35	9.338 635 78
2048	9.259 260 93	9.295 920 75	9.338 633 85
∞	9.259 260 4(3)	9.295 919 9(8)	9.338 633 8(5)
		$Q_5 \cdot 10^3 \equiv \left\langle \sum_{x,a} \frac{1}{m_x} p_x^i \left(\frac{\delta^{ij}}{r_{xa}} + \frac{r_{xa}^i\, r_{xa}^j}{r_{xa}^3}\right) p_a^j \right\rangle \cdot 10^3$	
128	−2.716 776 047	−2.042 822 31	−1.366 068 739 2
256	−2.716 927 777	−2.042 866 09	−1.366 118 195 7
512	−2.716 935 841	−2.041 645 96	−1.366 122 927 0
1024	−2.716 937 305	−2.041 636 68	−1.366 123 709 8
2048	−2.716 937 559	−2.041 636 65	−1.366 123 825 7
∞	−2.716 937 60(3)	−2.041 636 64(2)	−1.366 123 843(12)
		$Q_6 \cdot 10^6 \equiv \left\langle \frac{1}{m_0\, m_1} p_0^i \left(\frac{\delta^{ij}}{r_{01}} + \frac{r_{01}^i\, r_{01}^j}{r_{01}^3}\right) p_1^j \right\rangle \cdot 10^6$	
128	−3.664 977 870	−2.134 860 197	−1.320 794 344
256	−3.665 183 601	−2.135 316 159	−1.321 343 200
512	−3.665 198 266	−2.135 382 240	−1.321 371 779
1024	−3.665 200 088	−2.135 382 951	−1.321 373 805
2048	−3.665 200 016	−2.135 382 894	−1.321 373 947
∞	−3.665 200 01(4)	−2.135 382 90(3)	−1.321 373 958(12)
		$E_{\rm rel}$	
128	−0.204 529 420	−0.204 653 416	−0.204 793 910 0
256	−0.204 549 386	−0.204 659 239	−0.204 804 113 0
512	−0.204 548 291	−0.204 661 588	−0.204 805 591 2
1024	−0.204 547 896	−0.204 661 322	−0.204 805 225 9
2048	−0.204 547 619	−0.204 661 263	−0.204 805 181 5
∞	−0.204 547 56(4)	−0.204 661 246(17)	−0.204 805 172(7)