THE JOURNAL OF PHYSICAL CHEMISTRY A
J. Phys. Chem. A, 1998, 102(50), 10348-10357, DOI:10.1021/jp9824712

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Table 1S. Geometrical parameters for 2H-ANTA.[a]

Parameter	HF 6-31G**	HF 6-311+G**	MP2 6-31G**	MP2 6-311G**	MP2 6-311+G**	B3LYP 6-31G**	B3LYP 6-311+G**	BLYP 6-31G**	BLYP 6-311+G**	Exp. Ref.5	Exp. Ref.6
$r(N_1\text{-}N_2)$	1.3466 (.6)	1.3456 (.6)	1.3581 (.3)	1.3538 (.0)	1.3541	1.3615 (.6)	1.3594 (.4)	1.3787 (1.8)	1.3763 (1.6)	1.3687	1.3673
$r(N_2\text{-}C_3)$	1.3392 (1.5)	1.3390 (1.5)	1.3589 (.0)	1.3588 (.0)	1.3592	1.3633 (.3)	1.3625 (.2)	1.3783 (1.4)	1.3777 (1.4)	1.3499	1.3506
$r(C_3\text{-}N_4)$	1.3014 (2.0)	1.2999 (2.1)	1.3298 (.1)	1.3270 (.1)	1.3285	1.3237 (.4)	1.3204 (.6)	1.3373 (.7)	1.3335 (.4)	1.3336	1.3406
$r(N_4\text{-}C_5)$	1.3419 (.7)	1.3417 (.8)	1.3529 (.1)	1.3514 (.0)	1.3520	1.3545 (.2)	1.3521 (.0)	1.3673 (1.1)	1.3641 (.9)	1.3439	1.3412
$r(C_5\text{-}N_1)$	1.2801 (3.8)	1.2766 (4.1)	1.3345 (.3)	1.3303 (.0)	1.3308	1.3171 (1.0)	1.3116 (1.4)	1.3355 (.4)	1.3293 (.1)	1.3085	1.3012
$r(C_5\text{-}N_6)$	1.4523 (.3)	1.4593 (.1)	1.4523 (.3)	1.4589 (.1)	1.4573	1.4619 (.3)	1.4689 (.8)	1.4756 (1.3)	1.4829 (1.8)	1.4467	1.4452
$r(N_6\text{-}O_7)$	1.1900 (3.3)	1.1835 (3.9)	1.2415 (.9)	1.2285 (.2)	1.2310	1.2275 (.3)	1.2210 (.8)	1.2479 (1.4)	1.2418 (.9)	1.2256	1.2224
$r(N_6\text{-}O_8)$	1.1884 (3.5)	1.1822 (4.0)	1.2414 (.9)	1.2285 (.2)	1.2310	1.2265 (.4)	1.2202 (.9)	1.2468 (1.3)	1.2410 (.8)	1.2205	1.2251
$r(C_3\text{-}N_9)$	1.3599 (1.6)	1.3616 (1.5)	1.3830 (.0)	1.3830 (.0)	1.3825	1.3721 (.7)	1.3693 (1.0)	1.3843 (.1)	1.3803 (.2)	1.3408	1.3330
$r(N_9\text{-}H_{10})$	.9950 (1.7)	.9954 (1.7)	1.0106 (.2)	1.0117 (.1)	1.0123	1.0110 (.1)	1.0093 (.3)	1.0199 (.7)	1.0173 (.5)	0.8819	0.8559
$r(N_9\text{-}H_{11})$	.9957 (1.7)	.9961 (1.6)	1.0109 (.2)	1.0121 (.1)	1.0127	1.0115 (.1)	1.0101 (.3)	1.0200 (.7)	1.0180 (.5)	0.8743	0.8330
$r(N_2\text{-}H_{12})$	.9929 (1.8)	.9930 (1.8)	1.0087 (.3)	1.0101 (.1)	1.0112	1.0095 (.2)	1.0091 (.2)	1.0179 (.7)	1.0172 (.6)	0.8437	0.8496
$\theta(N_1\text{-}N_2\text{-}C_3)$	109.90 (1.1)	109.80 (1.2)	111.27 (.2)	111.13 (.0)	111.09	110.49 (.5)	110.31 (.7)	110.61 (.4)	110.39 (.6)	110.61	110.66
$\theta(N_2\text{-}C_3\text{-}N_4)$	109.90 (.1)	109.89 (.1)	109.75 (.0)	109.77 (.0)	109.76	109.67 (.1)	109.51 (.2)	109.73 (.0)	109.52 (.2)	109.52	109.01
$\theta(C_3\text{-}N_4\text{-}C_5)$	101.65 (.2)	101.66 (.2)	101.46 (.0)	101.44 (.0)	101.47	101.76 (.3)	102.04 (.6)	101.72 (.2)	102.09 (.6)	101.47	101.58
$\theta(N_4\text{-}C_5\text{-}N_1)$	117.43 (.2)	117.39 (.2)	117.79 (.1)	117.74 (.1)	117.66	117.62 (.0)	117.36 (.3)	117.87 (.2)	117.53 (.1)	118.32	118.39
$\theta(C_5\text{-}N_1\text{-}N_2)$	101.11 (1.1)	101.25 (1.2)	99.72 (.3)	99.92 (.1)	100.03	100.46 (.4)	100.78 (.7)	100.08 (.1)	100.47 (.4)	100.08	100.36
$\theta(N_1\text{-}C_5\text{-}N_6)$	120.78 (.3)	120.85 (.4)	120.28 (.1)	120.34 (.0)	120.39	120.45 (.0)	120.62 (.2)	120.25 (.1)	120.46 (.1)	120.97	120.18
$\theta(N_4\text{-}C_5\text{-}N_6)$	121.79 (.1)	121.76 (.2)	121.93 (.0)	121.92 (.0)	121.95	121.93 (.0)	122.02 (.1)	121.88 (.1)	122.01 (.0)	120.71	121.43
$\theta(C_5\text{-}N_6\text{-}O_7)$	117.00 (.1)	117.04 (.1)	116.87 (.1)	116.76 (.1)	116.93	117.02 (.1)	117.14 (.2)	117.00 (.1)	117.17 (.2)	118.16	117.54
$\theta(C_5\text{-}N_6\text{-}O_8)$	116.63 (.1)	116.55 (.0)	116.69 (.2)	116.60 (.1)	116.51	116.68 (.1)	116.63 (.1)	116.67 (.1)	116.66 (.1)	117.74	117.59
$\theta(O_7\text{-}N_6\text{-}O_8)$	126.37 (.1)	126.41 (.1)	126.44 (.1)	126.64 (.1)	126.56	126.29 (.2)	126.23 (.3)	126.33 (.2)	126.17 (.3)	124.10	124.87
$\theta(N_2\text{-}C_3\text{-}O_9)$	123.99 (.4)	123.97 (.4)	123.48 (.0)	123.53 (.0)	123.51	124.21 (.6)	124.34 (.7)	124.19 (.6)	124.38 (.7)	124.17	124.74
$\theta(N_4\text{-}C_3\text{-}O_9)$	126.07 (.4)	126.10 (.4)	126.60 (.0)	126.55 (.0)	126.59	126.04 (.4)	126.06 (.4)	125.96 (.5)	125.99 (.5)	125.54	126.24
$\theta(C_3\text{-}N_9\text{-}H_{10})$	117.23 (2.4)	116.83 (2.1)	114.23 (.2)	113.84 (.5)	114.43	116.66 (1.9)	117.49 (2.7)	116.08 (1.4)	117.29 (2.5)	119.00	120.09
$\theta(C_3\text{-}N_9\text{-}H_{11})$	113.45 (2.4)	113.45 (2.3)	110.18 (.6)	110.09 (.7)	110.84	112.33 (1.3)	113.46 (2.4)	111.69 (.8)	113.22 (2.1)	114.23	117.25

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Table 1S (continued)

$\theta(H_{10}\text{-}N_9\text{-}H_{11})$	114.14 (2.6)	113.77 (2.3)	110.87 (.3)	110.88 (.3)	111.20	113.09 (1.7)	113.78 (2.3)	112.33 (1.0)	113.40 (2.0)	121.64	122.27
$\theta(N_1\text{-}N_2\text{-}H_{12})$	120.23 (.6)	120.25 (.6)	119.47 (.1)	119.39 (.1)	119.54	119.55 (.0)	119.55 (.0)	119.23 (.3)	119.22 (.3)	118.06	117.11
$\theta(C_3\text{-}N_2\text{-}H_{12})$	129.74 (.4)	129.82 (.4)	129.21 (.1)	129.42 (.1)	129.28	129.87 (.5)	130.07 (.6)	130.07 (.6)	130.32 (.8)	131.11	131.95
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_4)$	-.26	-.14	0.69	.54	.86	.05	.08	.11	.10	0.33	0.37
$\tau(N_2\text{-}C_3\text{-}N_4\text{-}C_5)$	.38	.26	-.08	-.08	-.37	.21	.16	.19	.14	-0.38	-0.33
$\tau(C_3\text{-}N_4\text{-}C_5\text{-}N_6)$	179.93	179.81	-179.80	-179.96	179.72	179.99	179.99	179.99	179.89	179.30	-179.96
$\tau(N_1\text{-}C_5\text{-}N_6\text{-}O_7)$	-2.58	-7.31	-3.58	-3.69	-22.25	-1.32	-2.29	-1.47	-2.49	-11.05	-0.29
$\tau(N_4\text{-}C_5\text{-}N_6\text{-}O_8)$	-3.00	-7.59	-4.53	-4.28	-22.48	-1.79	-2.63	-1.97	-2.80	-9.94	0.38
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_9)$	177.50	177.45	176.27	176.38	176.71	176.86	176.86	176.37	176.53	-177.46	179.34
$\tau(N_2\text{-}C_3\text{-}N_9\text{-}H_{10})$	35.27	35.46	52.44	50.36	50.74	39.10	35.81	40.81	36.52	-18.62	8.07
$\tau(N_4\text{-}C_3\text{-}N_9\text{-}H_{11})$	-10.90	-11.98	-7.19	-9.31	-7.40	-11.72	-11.68	-13.01	-12.61	8.82	-0.13
$\tau(C_5\text{-}N_1\text{-}N_2\text{-}H_{12})$	176.19	176.22	176.58	176.52	175.86	176.68	176.89	176.63	176.79	-175.31	-174.85

[a] The values in parenthesis correspond to percentage differences relative to MP2/6-311+G** results.

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Table 2S. Geometrical parameters for 1H-ANTA.[a]

Parameter	HF 6-31G**	HF 6-311+G**	MP2 6-31G**	MP2 6-311G**	MP2 6-311+G**	B3LYP 6-31G**	B3LYP 6-311+G**	BLYP 6-31G**	BLYP 6-311+G**
$r(N_1\text{-}N_2)$	1.3456 (.0)	1.3448 (.1)	1.3509 (.4)	1.3463 (.0)	1.3460	1.3539 (.6)	1.3525 (.5)	1.3688 (1.7)	1.3665 (1.5)
$r(N_2\text{-}C_3)$	1.3039 (3.4)	1.3007 (3.6)	1.3520 (.2)	1.3480 (.1)	1.3499	1.3435 (.5)	1.3389 (.8)	1.3637 (1.0)	1.3589 (.7)
$r(C_3\text{-}N_4)$	1.3568 (.3)	1.3578 (.2)	1.3616 (.1)	1.3606 (.0)	1.3602	1.3644 (.3)	1.3631 (.2)	1.3755 (1.1)	1.3730 (0.9)
$r(N_4\text{-}C_5)$	1.2864 (2.8)	1.2837 (3.0)	1.3249 (.1)	1.3214 (.1)	1.3233	1.3157 (.6)	1.3113 (.9)	1.3314 (.6)	1.3267 (.3)
$r(C_5\text{-}N_1)$	1.3130 (2.6)	1.3126 (2.6)	1.3475 (.0)	1.3469 (.1)	1.3480	1.3416 (.5)	1.3398 (.6)	1.3578 (.7)	1.3561 (.6)
$r(C_5\text{-}N_6)$	1.4454 (.1)	1.4529 (.6)	1.4373 (.5)	1.4438 (.0)	1.4439	1.4450 (.1)	1.4524 (.6)	1.4547 (.7)	1.4616 (1.2)
$r(N_6\text{-}O_7)$	1.1979 (3.2)	1.1919 (3.7)	1.2489 (.9)	1.2358 (.2)	1.2380	1.2380 (.0)	1.2322 (.5)	1.2609 (1.8)	1.2555 (1.4)
$r(N_6\text{-}O_8)$	1.1811 (3.8)	1.1740 (4.4)	1.2397 (.9)	1.2261 (.2)	1.2282	1.2217 (.5)	1.2146 (1.1)	1.2428 (1.2)	1.2362 (.7)
$r(C_3\text{-}N_9)$	1.3639 (1.1)	1.3660 (0.9)	1.3785 (.0)	1.3795 (.0)	1.3791	1.3697 (.7)	1.3679 (.8)	1.3796 (.0)	1.3765 (.2)
$r(N_9\text{-}H_{10})$	.9944 (1.6)	0.9950 (1.6)	1.0088 (.2)	1.0102 (.1)	1.0110	1.0094 (.2)	1.0083 (.3)	1.0178 (.7)	1.0160 (.5)
$r(N_9\text{-}H_{11})$	.9943 (1.6)	0.9949 (1.6)	1.0085 (.2)	1.0099 (.1)	1.0107	1.0092 (.2)	1.0082 (.3)	1.0176 (.7)	1.0158 (.5)
$r(N_1\text{-}H_{12})$	.9934 (1.9)	0.9937 (1.8)	1.0094 (.3)	1.0109 (.1)	1.0123	1.0099 (.2)	1.0098 (.3)	1.0179 (.6)	1.0177 (.5)
$\theta(N_1\text{-}N_2\text{-}C_3)$	102.69 (.9)	102.89 (1.1)	101.44 (.3)	101.59 (.2)	101.77	101.80 (.0)	102.19 (.4)	101.24 (.5)	101.73 (.0)
$\theta(N_2\text{-}C_3\text{-}N_4)$	114.64 (.7)	114.50 (.8)	115.68 (.2)	115.64 (.2)	115.44	115.20 (.2)	114.79 (.6)	115.63 (.2)	115.09 (.3)
$\theta(C_3\text{-}N_4\text{-}C_5)$	101.40 (.0)	101.42 (.0)	101.29 (.1)	101.25 (.1)	101.39	101.53 (.1)	101.85 (.4)	101.45 (.1)	101.90 (.5)
$\theta(N_4\text{-}C_5\text{-}N_1)$	112.91 (1.1)	112.99 (1.2)	111.74 (.0)	111.76 (.1)	111.69	112.01 (.3)	111.97 (.3)	111.87 (.2)	111.75 (.1)
$\theta(C_5\text{-}N_1\text{-}N_2)$	108.36 (1.2)	108.20 (1.4)	109.85 (.1)	109.76 (.0)	109.71	109.46 (.2)	109.20 (.5)	109.81 (.1)	109.53 (.2)
$\theta(N_1\text{-}C_5\text{-}N_6)$	120.84 (.1)	120.92 (.0)	120.64 (.3)	120.63 (.3)	120.95	120.67 (.2)	120.96 (.0)	120.58 (.3)	121.00 (.0)
$\theta(N_4\text{-}C_5\text{-}N_6)$	126.25 (.9)	126.08 (1.0)	127.62 (.2)	127.61 (.2)	127.36	127.31 (.0)	127.06 (.2)	127.55 (.1)	127.25 (.1)
$\theta(C_5\text{-}N_6\text{-}O_7)$	115.09 (.3)	115.17 (.2)	115.22 (.1)	115.21 (.2)	115.38	115.18 (.2)	115.36 (.0)	115.18 (.2)	115.44 (.1)
$\theta(C_5\text{-}N_6\text{-}O_8)$	117.95 (.0)	117.85 (.1)	118.10 (.1)	117.98 (.0)	117.98	118.24 (.2)	118.18 (.2)	118.29 (.3)	118.27 (.2)
$\theta(O_7\text{-}N_6\text{-}O_8)$	126.96 (.3)	126.98 (.3)	126.68 (.0)	126.82 (.1)	126.64	126.58 (.0)	126.46 (.1)	126.53 (.1)	126.29 (.3)
$\theta(N_2\text{-}C_3\text{-}O_9)$	123.75 (1.3)	123.89 (1.4)	122.04 (.1)	122.13 (.0)	122.13	122.56 (.4)	122.83 (.6)	122.05 (.1)	122.36 (.2)
$\theta(N_4\text{-}C_3\text{-}O_9)$	121.59 (.6)	121.58 (.6)	122.15 (.1)	122.14 (.1)	122.31	122.19 (.1)	122.33 (.0)	122.26 (.0)	122.49 (.1)
$\theta(C_3\text{-}N_9\text{-}H_{10})$	115.28 (1.4)	115.04 (1.2)	113.38 (.2)	112.91 (.6)	113.65	115.40 (1.5)	116.18 (2.2)	115.08 (1.3)	116.27 (2.3)

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Table 2S (continued)

$\theta(C_3\text{-}N_9\text{-}H_{11})$	114.83 (1.6)	114.59 (1.4)	112.76 (.3)	112.29 (.7)	113.04	114.74 (1.5)	115.51 (2.2)	114.39 (1.2)	115.57 (2.2)
$\theta(H_{10}\text{-}N_9\text{-}H_{11})$	114.98 (1.7)	114.48 (1.3)	112.98 (.1)	112.82 (.2)	113.04	115.05 (1.8)	115.50 (2.2)	114.58 (1.4)	115.44 (2.1)
$\theta(N_2\text{-}N_1\text{-}H_{12})$	122.81 (.7)	122.70 (.6)	122.25 (.3)	121.98 (.0)	121.94	122.63 (.6)	122.26 (.3)	122.57 (.5)	122.02 (.1)
$\theta(C_5\text{-}N_1\text{-}H_{12})$	128.82 (.4)	129.10 (.6)	127.91 (.3)	128.26 (.1)	128.35	127.92 (.3)	128.54 (.1)	127.62 (.6)	128.45 (.1)
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_4)$	-.47	-.38	-.20	-.27	-.06	-.42	-.27	-.45	-.30
$\tau(N_2\text{-}C_3\text{-}N_4\text{-}C_5)$	.37	.30	.13	.19	.05	.31	.22	.33	.26
$\tau(C_3\text{-}N_4\text{-}C_5\text{-}N_6)$	-180.00	-179.87	-179. 71	-179.76	-179.37	-179.93	-179.80	-179.89	-179.81
$\tau(N_1\text{-}C_5\text{-}N_6\text{-}O_7)$	.62	.45	0.71	0.66	0.67	0.33	0.29	0.29	.26
$\tau(N_4\text{-}C_5\text{-}N_6\text{-}O_8)$	.59	.29	.30	.43	.06	.30	.04	.17	.00
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_9)$	177.54	177.33	175.89	176.17	175.86	177.11	177.15	176.73	176.90
$\tau(N_2\text{-}C_3\text{-}N_9\text{-}H_{10})$	20.49	21.34	25.68	25.83	25.76	21.76	20.56	22.91	20.89
$\tau(N_4\text{-}C_3\text{-}N_9\text{-}H_{11})$	-24.49	-25.31	-28.49	-29.02	-28.00	-23.59	-22.19	-24.33	-22.01
$\tau(H_{12}\text{-}N_1\text{-}N_2\text{-}C_3)$	-179.62	-179.77	-179.98	-179.89	179.80	-179.84	-179.95	-179.92	-179.95

[a] The values in parenthesis correspond to percentage differences relative to MP2/6-311+G** results

Table 3S. Geometrical parameters for 3H-ANTA.[a]

Parameter	HF 6-31G**	HF 6-311+G**	MP2 6-31G**	MP2 6-311G**	MP2 6-311+G**	B3LYP 6-31G**	B3LYP 6-311+G**	BLYP 6-31G**	BLYP 6-311+G**
$r(N_1\text{-}N_2)$	1.3562 (1.5)	1.3571 (1.5)	1.3819 (.3)	1.3774 (.0)	1.3771	1.3690 (.6)	1.3666 (.8)	1.3869 (.7)	1.3828 (.4)
$r(N_2\text{-}C_3)$	1.2971 (2.2)	1.2938 (2.5)	1.3293 (.2)	1.3248 (.2)	1.3268	1.3313 (.3)	1.3269 (.0)	1.3487 (1.7)	1.3444 (1.3)
$r(C_3\text{-}N_4)$	1.3473 (1.4)	1.3487 (1.3)	1.3657 (.1)	1.3658 (.1)	1.3666	1.3614 (.4)	1.3612 (.4)	1.3733 (.5)	1.3730 (.5)
$r(N_4\text{-}C_5)$	1.3599 (.0)	1.3599 (.0)	1.3594 (.1)	1.3591 (.1)	1.3605	1.3735 (1.0)	1.3734 (1.0)	1.3865 (1.9)	1.3869 (1.9)
$r(C_5\text{-}N_1)$	1.2675 (3.6)	1.2632 (3.9)	1.3183 (.3)	1.3135 (.1)	1.3149	1.3050 (.8)	1.2992 (1.2)	1.3228 (.6)	1.3170 (.2)
$r(C_5\text{-}N_6)$	1.4317 (1.0)	1.4392 (.5)	1.4395 (.5)	1.4466 (.0)	1.4467	1.4338 (.9)	1.4387 (.6)	1.4445 (.2)	1.4488 (.1)
$r(N_6\text{-}O_7)$	1.1824 (3.5)	1.1748 (4.1)	1.2370 (.9)	1.2235 (.2)	1.2254	1.2229 (.2)	1.2159 (.8)	1.2438 (1.5)	1.2373 (1.0)
$r(N_6\text{-}O_8)$	1.2010 (3.0)	1.1955 (3.4)	1.2480 (.8)	1.2352 (.2)	1.2379	1.2418 (.3)	1.2369 (.1)	1.2648 (2.2)	1.2609 (1.9)
$r(C_3\text{-}N_9)$	1.3650 (1.4)	1.3663 (1.3)	1.3848 (.1)	1.3852 (.1)	1.3839	1.3701 (1.0)	1.3670 (1.2)	1.3804 (.3)	1.3761 (.6)
$r(N_9\text{-}H_{10})$	.9969 (1.7)	.9971 (1.7)	1.0120 (.2)	1.0133 (.1)	1.0139	1.0122 (.2)	1.0108 (.3)	1.0207 (.7)	1.0187 (.5)
$r(N_9\text{-}H_{11})$	.9963 (1.7)	.9966 (1.6)	1.0117 (.2)	1.0129 (.0)	1.0133	1.0113 (.2)	1.0095 (.4)	1.0198 (.6)	1.0173 (.4)
$r(N_4\text{-}H_{12})$	.9940 (1.8)	.9941 (1.8)	1.0091 (.3)	1.0105 (.1)	1.0120	1.0099 (.2)	1.0098 (.2)	1.0181 (.6)	1.0179 (.6)
$\theta(N_1\text{-}N_2\text{-}C_3)$	107.55 (.3)	107.57 (.2)	107.81 (.0)	107.83 (.0)	107.83	107.59 (.2)	107.66 (.2)	107.48 (.3)	107.56 (.2)
$\theta(N_2\text{-}C_3\text{-}N_4)$	110.56 (.2)	110.58 (.2)	110.29 (.1)	110.36 (.0)	110.36	110.31 (.0)	110.23 (.1)	110.39 (.0)	110.27 (.1)
$\theta(C_3\text{-}N_4\text{-}C_5)$	102.89 (.6)	102.73 (.8)	103.80 (.3)	103.54 (.0)	103.53	103.54 (.0)	103.47 (.1)	103.70 (.2)	103.66 (.1)
$\theta(N_4\text{-}C_5\text{-}N_1)$	112.05 (.4)	112.18 (.2)	112.43 (.0)	112.48 (.0)	112.45	111.77 (.6)	111.72 (.7)	111.81 (.6)	111.67 (.7)
$\theta(C_5\text{-}N_1\text{-}N_2)$	106.95 (1.1)	106.93 (1.0)	105.67 (.2)	105.79 (.0)	105.83	106.78 (.9)	106.91 (1.0)	106.62 (.7)	106.83 (.9)
$\theta(N_1\text{-}C_5\text{-}N_6)$	127.12 (.1)	126.91 (.1)	127.27 (.2)	127.23 (.2)	127.01	127.82 (.6)	127.56 (.4)	128.02 (.8)	127.70 (.5)
$\theta(N_4\text{-}C_5\text{-}N_6)$	120.83 (.3)	120.90 (.3)	120.29 (.2)	120.28 (.2)	120.51	120.40 (.1)	120.72 (.2)	120.17 (.3)	120.62 (.1)
$\theta(C_5\text{-}N_6\text{-}O_7)$	118.51 (.3)	118.49 (.3)	118.13 (.0)	118.00 (.1)	118.13	118.72 (.5)	118.83 (.6)	118.74 (.5)	118.92 (.7)
$\theta(C_5\text{-}N_6\text{-}O_8)$	114.93 (.2)	114.93 (.2)	115.14 (.0)	115.12 (.0)	115.18	114.98 (.2)	115.06 (.1)	114.97 (.2)	115.10 (.1)
$\theta(O_7\text{-}N_6\text{-}O_8)$	126.56 (.1)	126.58 (.1)	126.73 (.0)	126.88 (.1)	126.69	126.29 (.3)	126.11 (.5)	126.29 (.3)	125.98 (.6)
$\theta(N_2\text{-}C_3\text{-}O_9)$	125.83 (.3)	125.92 (.2)	126.31 (.1)	126.31 (.1)	126.23	125.04 (.9)	125.07 (.9)	124.76 (1.2)	124.76 (1.2)
$\theta(N_4\text{-}C_3\text{-}O_9)$	123.56 (.3)	123.43 (.2)	123.22 (.0)	123.17 (.0)	123.21	124.55 (1.1)	124.60 (1.1)	124.73 (1.2)	124.86 (1.3)
$\theta(C_3\text{-}N_9\text{-}H_{10})$	112.30 (2.0)	112.36 (2.1)	109.34 (.7)	109.19 (.8)	110.07	111.93 (1.7)	113.14 (2.8)	111.54 (1.3)	113.11 (2.8)
$\theta(C_3\text{-}N_9\text{-}H_{11})$	116.06 (1.8)	115.78 (1.5)	113.67 (.3)	113.25 (.7)	114.04	116.74 (2.4)	117.62 (3.1)	116.54 (2.2)	117.80 (3.3)

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Table 3S (continued)

$\theta(H_{10}\text{-}N_9\text{-}H_{11})$	112.95 (2.2)	112.66 (1.9)	110.15 (.4)	110.09 (.4)	110.57	113.06 (2.2)	113.77 (2.9)	112.63 (1.9)	113.72 (2.8)
$\theta(C_3\text{-}N_4\text{-}H_{12})$	130.17 (.3)	130.07 (.2)	130.21 (.3)	130.10 (.2)	129.83	131.24 (1.1)	130.79 (.7)	131.71 (1.4)	131.05 (.9)
$\theta(C_4\text{-}N_4\text{-}H_{12})$	126.71 (.3)	126.95 (.5)	125.83 (.4)	126.21 (.1)	126.35	125.10 (1.0)	125.61 (.6)	124.49 (1.5)	125.18 (.9)
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_4)$	-.67	-.63	-.22	-.35	-.34	-.45	-.38	-.35	-.37
$\tau(N_2\text{-}C_3\text{-}N_4\text{-}C_5)$	.53	.52	-.01	.07	.29	.27	.27	.18	.26
$\tau(C_3\text{-}N_4\text{-}C_5\text{-}N_6)$	-179.75	-179.69	-178.65	-178.97	-178.44	-179.45	-179.33	-179.36	-179.30
$\tau(N_1\text{-}C_5\text{-}N_6\text{-}O_7)$	.22	.23	.90	.54	.79	.42	.62	.45	.66
$\tau(N_4\text{-}C_5\text{-}N_6\text{-}O_8)$	-.38	-.50	-.64	-.55	-1.49	-.38	-.41	-.40	-.42
$\tau(N_1\text{-}N_2\text{-}C_3\text{-}N_9)$	176.63	176.46	174.83	175.08	174.66	176.12	176.12	175.77	175.95
$\tau(N_2\text{-}C_3\text{-}N_9\text{-}H_{10})$	7.20	8.14	2.73	3.14	3.59	10.06	10.16	11.64	11.23
$\tau(N_4\text{-}C_3\text{-}N_9\text{-}H_{11})$	-43.80	-43.74	-59.28	-58.93	-57.08	-41.35	-37.84	-41.52	-36.96
$\tau(C_5\text{-}N_1\text{-}N_2\text{-}H_{12})$	175.20	174.98	175.66	175.77	174.29	176.25	176.35	176.52	176.52

[a] The values in parenthesis correspond to percentage differences relative to MP2/6-311+G** results

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Table 4S. Scaled harmonic vibrational frequencies (cm^{-1}) for 2H-ANTA molecules.[a]

Mode	MP2			B3LYP		BLYP		Assignment[b]
	6-31G**	6-311G**	6-311+G**	6-31G**	6-311+G**	6-31G**	6-311+G**	
ν_1	27.45 (32.2)	24.42 (39.7)	40.51	42.22 (4.2)	32.65 (19.4)	45.07 (11.3)	33.12 (18.2)	NO_2 torsion
ν_2	153.04 (2.0)	159.26 (6.1)	150.08	163.14 (8.7)	160.79 (7.1)	160.02 (6.6)	157.55 (5.0)	skeletal def
ν_3	191.00 (.7)	93.84 (.8)	192.33	197.79 (2.8)	196.69 (2.3)	196.30 (2.1)	195.34 (1.6)	NO_2 rock
ν_4	206.51 (.9)	211.08 (3.1)	204.63	257.73 (25.9)	253.03 (23.7)	265.92 (30.0)	259.90 (27.0)	NH_2 rock
ν_5	307.57 (2.2)	318.73 (5.9)	301.08	328.94 (9.3)	326.14 (8.3)	322.41 (7.1)	320.09 (6.3)	skeletal def
ν_6	366.21 (1.0)	368.88 (.3)	369.99	374.79 (1.3)	374.31 (1.2)	370.61 (.2)	369.98 (.0)	ring def
ν_7	409.04 (.2)	412.93 (1.1)	408.37	414.78 (1.6)	411.35 (.7)	406.19 (.5)	402.86 (1.4)	C-NO_2 def
ν_8	499.63 (9.7)	484.82 (6.5)	455.41	479.27 (5.2)	484.72 (6.4)	451.19 (.9)	458.55 (.7)	NO_2 def
ν_9	525.41 (1.7)	534.39 (3.4)	516.66	539.60 (4.4)	538.52 (4.2)	533.74 (3.3)	533.48 (3.3)	NH_2 def
ν_{10}	607.73 (1.9)	617.59 (.3)	619.48	582.24 (6.0)	547.71 (11.6)	604.66 (2.4)	559.90 (9.6)	ring torsion+NO_2 def
ν_{11}	635.89 (.2)	647.80 (2.1)	634.64	633.52 (.2)	633.97 (.1)	624.96 (1.5)	625.17 (1.5)	ring torsion
ν_{12}	679.89 (3.0)	704.36 (.5)	701.11	707.72 (.9)	709.48 (1.2)	696.83 (.6)	696.67 (.6)	ring+NO_2+NH_2 def
ν_{13}	692.64 (1.8)	718.77 (1.9)	705.66	722.60 (2.4)	722.52 (2.4)	719.12 (1.9)	717.71 (1.7)	ring torsion
ν_{14}	726.13 (.6)	747.13 (2.3)	730.15	749.39 (2.6)	754.60 (3.3)	729.41 (.1)	736.79 (.9)	ring torsion
ν_{15}	784.23 (3.0)	812.03 (.5)	808.07	817.80 (1.2)	824.72 (2.1)	800.04 (1.0)	805.72 (.3)	NO_2 def+ring def
ν_{16}	949.67 (1.2)	962.83 (.2)	961.19	981.82 (2.1)	980.10 (2.0)	965.90 (.5)	964.63 (.4)	N_4-C_5-N_1 bend
ν_{17}	1002.40 (.7)	1010.99 (.1)	1009.59	1009.12 (.0)	1003.03 (.6)	998.39 (1.1)	990.83 (1.9)	N_1-N_2-C_3 bend
ν_{18}	1076.12 (.2)	1081.98 (.3)	1078.54	1076.78 (.2)	1069.86 (.8)	1071.04 (.7)	1062.20 (1.5)	ring def
ν_{19}	1143.10 (1.2)	1158.87 (.2)	1156.68	1124.26 (2.8)	1117.11 (3.4)	1095.43 (5.3)	1087.71 (6.0)	N-N sym str
ν_{20}	1257.97 (.8)	1274.38 (.5)	1267.54	1298.90 (2.5)	1288.05 (1.6)	1271.75 (.3)	1254.886(1.0)	NO_2-sym. str
ν_{21}	1286.10 (.1)	1291.00 (.3)	1287.63	1307.87 (1.6)	1299.04 (.9)	1289.32 (.1)	1277.75 (.8)	ring def+N-H bend
ν_{22}	1372.82 (.1)	1378.61 (.3)	1374.48	1367.81 (.5)	1341.41 (2.4)	1304.58 (5.1)	1284.81 (6.5)	C-NO_2 sym str
ν_{23}	1402.41 (.1)	1409.50 (.4)	1404.07	1413.91 (.7)	1400.13 (.3)	1388.56 (1.1)	1376.39 (2.0)	ring def
ν_{24}	1451.54 (.1)	1462.21 (.6)	1453.28	1494.00 (2.8)	1482.57 (2.0)	1451.68 (.1)	1438.00 (1.1)	C-N sym str

Table 4S (continued)

ν_{25}	1535.36 (.3)	1534.78 (.2)	1531.08	1553.30 (1.5)	1544.38 (.9)	1520.86 (.7)	1469.79 (4.0)	C-NH_2 assymstr+NH2 bend
ν_{26}	1594.88 (.3)	1593.81 (.2)	1590.37	1599.81 (.6)	1553.99 (2.3)	1550.35 (2.5)	1541.92 (3.0)	C-NH_2 symm str+NH2 bend
ν_{27}	1701.66 (.2)	1721.87 (1.3)	1699.00	1617.12 (4.8)	1606.17 (5.5)	1612.03 (5.1)	1604.92 (5.5)	N-O assym str
ν_{28}	3396.33 (.2)	3407.10 (.1)	3404.68	3438.03 (1.0)	3435.54 (.9)	3441.63 (1.1)	3450.01 (1.3)	N-H symm str (NH_2)
ν_{29}	3484.79 (.1)	3489.52 (.3)	3479.87	3516.61 (1.1)	3498.07 (.5)	3518.66 (1.1)	3505.30 (.7)	N-H str (N_1-H_{12})
ν_{30}	3504.42 (.0)	3507.00 (.0)	3505.55	3543.17 (1.1)	3532.62 (.8)	3546.50 (1.2)	3546.61 (1.2)	N-H assym str (NH_2)
rms	2.17	1.95	0.0	5.05	5.54	5.59	6.81	

[a]The values in parentheses correspond to percentage differences relative to MP2/6-311+G** frequencies.
[b]The assignment is based on the MP2/6-311+G** eigenvectors. The legened of abbreviations used in text is: def=deformation; str=strectching; assym=assymetric; symm=symmetric.

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Table 5S. Scaled harmonic vibrational frequencies (cm^{-1}) for 1H-ANTA and 3H-ANTA molecules.[a]

Mode	1H-ANTA					3H-ANTA				
	MP2/ 6-31G**	MP2/ 6-311G**	MP2/ 6-311+G**	B3LYP/ 6-311+G**	BLYP/ 6-311+G**	MP2/ 6-31G**	MP2/ 6-311G**	MP2/ 6-311+G**	B3LYP/ 6-311+G**	BLYP/ 6-311+G**
ν_1	70.84 (37.2)	67.85 (31.4)	51.65	71.56 (38.5)	72.94 (41.2)	67.88 (22.5)	66.28 (19.6)	55.42	82.00 (48.1)	82.48 (48.8)
ν_2	141.25 (2.2)	150.20 (8.7)	138.24	155.89 (12.8)	151.99 (9.9)	140.70 (1.0)	149.51 (7.4)	139.25	146.90 (5.5)	143.62 (3.1)
ν_3	185.28 (1.0)	186.39 (.4)	187.10	188.52 (.8)	187.35 (.1)	184.07 (1.1)	185.34 (.4)	186.17	188.88 (1.5)	187.77 (.9)
ν_4	269.33 (.8)	275.82 (3.2)	267.25	309.95 (16.0)	312.36 (16.9)	219.55 (1.5)	222.70 (.0)	222.80	260.80 (17.1)	275.78 (23.8)
ν_5	307.70 (.9)	320.93 (5.2)	304.98	336.34 (10.3)	339.00 (11.2)	291.05 (.2)	305.55 (4.8)	291.56	319.61 (9.6)	314.87 (8.0)
ν_6	371.32 (.7)	374.99 (.3)	373.81	380.56 (1.8)	378.48 (1.3)	357.23 (.9)	362.67 (.6)	360.42	370.94 (2.9)	368.18 (2.2)
ν_7	410.09 (.8)	415.61 (2.1)	406.92	414.75 (1.9)	409.56 (.7)	409.73 (.4)	413.19 (.4)	411.45	413.16 (.4)	406.14 (1.3)
ν_8	494.63 (19.2)	489.67 (18.0)	414.95	477.11 (15.0)	478.15 (15.2)	511.38 (9.5)	523.37 (12.1)	467.05	514.35 (10.1)	503.24 (7.7)
ν_9	528.94 (1.7)	539.01 (.1)	538.32	533.86 (0.8)	515.77 (4.2)	537.13 (.5)	547.84 (2.5)	534.59	545.06 (2.0)	538.49 (.7)
ν_{10}	602.66 (.7)	619.65 (3.6)	598.30	543.41 (9.2)	538.01 (10.1)	581.98 (1.8)	594.13 (3.9)	571.60	555.55 (2.8)	554.17 (3.0)
ν_{11}	619.50 (.2)	628.53 (1.6)	618.40	623.18 (.8)	618.44 (.0)	619.69 (1.3)	637.06 (4.1)	611.71	611.82 (.0)	602.94 (1.4)
ν_{12}	649.40 (2.1)	681.92 (7.2)	636.01	718.22 (12.9)	699.11 (9.9)	659.59 (1.2)	689.15 (5.8)	651.54	694.85 (6.6)	678.37 (4.1)
ν_{13}	684.67 (1.4)	704.65 (1.5)	694.48	725.20 (4.4)	713.90 (2.8)	686.75 (1.1)	697.53 (.5)	694.05	715.36 (3.1)	704.70 (1.5)
ν_{14}	718.84 (1.6)	740.70 (1.4)	730.42	737.46 (1 .0)	731.13 (.1)	756.62 (.5)	777.11 (3.2)	753.14	723.39 (4.0)	713.38 (5.3)
ν_{15}	780.86 (2.9)	807.16 (.4)	804.13	818.98 (1.8)	800.16 (.5)	771.68 (3.1)	799.76 (.4)	796.58	811.48 (1.9)	790.80 (.7)
ν_{16}	953.08 (1.2)	966.52 (.2)	964.41	976.95 (1.3)	962.85 (.2)	959.69 (1.2)	975.96 (.5)	971.42	984.80 (1.4)	973.09 (.2)
ν_{17}	999.93 (.8)	1011.34 (.3)	1008.36	1026.89 (1.8)	1015.57 (.7)	978.01 (.5)	986.40 (.4)	982.89	993.97 (1.1)	978.48 (.4)
ν_{18}	1051.39 (.4)	1059.78 (.4)	1055.34	1034.20 (2.0)	1026.14 (2.8)	1050.34 (.8)	1063.76 (.5)	1058.91	1046.72 (1.2)	1027.12 (3.0)
ν_{19}	1139.50 (1.3)	1152.19 (.2)	1154.71	1123.51 (2.7)	1098.80 (4.8)	1090.77 (.5)	1100.83 (.4)	1096.52	1070.21 (2.4)	1042.98 (4.9)
ν_{20}	1209.74 (1.0)	1225.64 (.3)	1222.44	1218.96 (.3)	1192.84 (2.4)	1127.12 (.4)	1134.73 (.3)	1131.58	1142.55 (1.0)	1126.04 (.5)
ν_{21}	1302.63 (.2)	1311.62 (.5)	1305.64	1319.65 (1.1)	1257.01 (3.7)	1296.41 (.1)	1308.93 (.9)	1297.41	1306.04 (.7)	1243.70 (4.1)
ν_{22}	1331.79 (.3)	1338.99 (.8)	1328.00	1324.48 (.3)	1301.60 (2.0)	1398.23 (.2)	1409.70 (.6)	1401.48	1337.21 (4.6)	1311.50 (6.4)
ν_{23}	1453.47 (.1)	1458.61 (.5)	1452.03	1434.09 (1.2)	1401.73 (3.5)	1412.14 (.3)	1418.55 (.8)	1407.70	1436.16 (2.0)	1394.42 (.9)
ν_{24}	1466.86 (.1)	1475.86 (.5)	1467.84	1479.64 (.8)	1454.72 (.9)	1460.46 (.1)	1469.95 (.5)	1462.62	1462.66 (.0)	1421.81 (2.8)
ν_{25}	1498.96 (.0)	1506.04 (.5)	1498.92	1521.99 (1.5)	1463.23 (2.4)	1521.92 (.3)	1522.72 (.3)	1517.41	1529.74 (.8)	1457.17 (4.0)

Table 5S (continued)

ν_{26}	1583.32 (.6)	1578.49 (.2)	1574.63	1545.66 (1.8)	1496.75 (4.9)	1587.54 (.5)	1582.25 (.2)	1579.85	1539.40 (2.6)	1525.59 (3.4)
ν_{27}	1689.72 (.1)	1710.77 (1.3)	1688.86	1590.66 (5.8)	1594.44 (5.6)	1691.26 (.2)	1712.14 (1.4)	1687.93	1598.95 (5.3)	1600.48 (5.2)
ν_{28}	3418.26 (.1)	3425.99 (.1)	3421.87	3451.94 (.9)	3470.38 (1.4)	3383.16 (.3)	3392.46 (.0)	3392.28	3429.57 (1.1)	3445.47 (1.6)
ν_{29}	3485.15 (.3)	3488.09 (.4)	3475.48	3501.30 (.7)	3514.12 (1.1)	3483.37 (.3)	3489.28 (.4)	3473.86	3493.66 (.6)	3501.95 (.8)
ν_{30}	3536.44 (.1)	3535.48 (.1)	3531.91	3557.42 (.7)	3576.62 (1.3)	3488.67 (.1)	3489.40 (.0)	3490.57	3526.35 (1.0)	3542.80 (1.5)
rms	3.10	3.39	0.0	6.17	7.43	2.02	3.03	0.0	5.60	7.12

[a]The values in parentheses correspond to percentage differences relative to MP2/6-311+G** frequencies.

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