Supplementary Material (ESI) for *PCCP*

Anomeric effect in N-azidomethylpyrrolidine: gas-phase electron diffraction and theoretical study

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Electronic supplementary information

Experimental conditions of gas-phase electron diffraction experiment (**Table S1**), experimental intensity curves with final backgrounds (**Table S2, Fig. S1, Fig. S2**), equilibrium distribution of AMP conformers (**Table S3**), molecular structure of *gauche-anti* conformer of AMP obtained by gas-phase electron diffraction and quantum chemical calculations (**Table S4**), molecular structure of *anti-gauche* conformer of AMP obtained by gas-phase electron diffraction and quantum chemical calculations (**Table S5**), vibrational amplitudes and vibrational corrections for non-hydrogen distances of *gauche-gauche* conformer calculated at different levels of theory (**Table S6**), vibrational amplitudes (u) and harmonic ($r_{h1} - r_a$) vibrational corrections obtained from the MP2/6-311+G(2df,p) force field for different conformers of AMP (**Table S7**), correlation matrix (**Table S8**), experimental coordinates of atoms for three conformers of AMP (**Table S9**).

Table S1 Experimental conditions of gas-phase electron diffraction experiment

	Long camera	Short camera
Camera distance (mm)	362.28	193.94
Nozzle temperature (K)	295	295
Accelerating voltage (kV)	60	60
Electron wavelength (Å)	0.049503	0.049566
Number of plates used	3	3
Range of s value ($Å^{-1}$) [a]	3.8-17.6	8.0-33.0
Scale factor	0.604(8) [b]	0.674(13) [b]

[a] $s=4\pi\lambda^{-1}\sin\theta/2$, where θ is the scattering angle and λ is the electron wavelength. [b] Value in parenthesis is the estimated standard deviation.

Table S2 Experimental intensity curves with backgrounds for AMP

s, Å^{-1}	Intensity	Background
Long camera		
3.8	0.4274	0.4727
4.0	0.4296	0.4810
4.2	0.4350	0.4894
4.4	0.4426	0.4964
4.6	0.4560	0.5018
4.8	0.4718	0.5055
5.0	0.4950	0.5075
5.2	0.5186	0.5076
5.4	0.5385	0.5053
5.6	0.5528	0.5011
5.8	0.5593	0.4955
6.0	0.5556	0.4893
6.2	0.5409	0.4825
6.4	0.5161	0.4750
6.6	0.4852	0.4668
6.8	0.4545	0.4581
7.0	0.4298	0.4493
7.2	0.4127	0.4406
7.4	0.4029	0.4322
7.6	0.3992	0.4241
7.8	0.3990	0.4166
8.0	0.4005	0.4094
8.2	0.4019	0.4023
8.4	0.4019	0.3954
8.6	0.3995	0.3885
8.8	0.3947	0.3818
9.0	0.3866	0.3756
9.2	0.3766	0.3700
9.4	0.3659	0.3649
9.6	0.3563	0.3603
9.8	0.3486	0.3559
10.0	0.3430	0.3515
10.2	0.3395	0.3473
10.4	0.3377	0.3433
10.6	0.3365	0.3397
10.8	0.3352	0.3364
11.0	0.3329	0.3333
11.2	0.3300	0.3303
11.4	0.3263	0.3271
11.6	0.3225	0.3238
11.8	0.3189	0.3206
12.0	0.3156	0.3173
12.2	0.3129	0.3142
12.4	0.3107	0.3112
12.6	0.3091	0.3083
12.8	0.3080	0.3054
13.0	0.3076	0.3027

13.2	0.3072	0.3001
13.4	0.3065	0.2976
13.6	0.3047	0.2952
13.8	0.3016	0.2929
14.0	0.2971	0.2906
14.2	0.2918	0.2884
14.4	0.2857	0.2861
14.6	0.2799	0.2840
14.8	0.2749	0.2821
15.0	0.2716	0.2804
15.2	0.2697	0.2790
15.4	0.2694	0.2779
15.6	0.2698	0.2769
15.8	0.2710	0.2760
16.0	0.2724	0.2752
16.2	0.2734	0.2744
16.4	0.2744	0.2739
16.6	0.2752	0.2734
16.8	0.2759	0.2732
17.0	0.2764	0.2732
17.2	0.2771	0.2734
17.4	0.2776	0.2737
17.6	0.2780	0.2740

Short camera

8.0	0.4223	0.4328
8.2	0.4261	0.4263
8.4	0.4284	0.4197
8.6	0.4273	0.4132
8.8	0.4215	0.4068
9.0	0.4125	0.4008
9.2	0.4012	0.3951
9.4	0.3908	0.3898
9.6	0.3805	0.3849
9.8	0.3721	0.3802
10.0	0.3660	0.3757
10.2	0.3621	0.3713
10.4	0.3604	0.3670
10.6	0.3588	0.3629
10.8	0.3572	0.3590
11.0	0.3544	0.3552
11.2	0.3513	0.3515
11.4	0.3472	0.3479
11.6	0.3431	0.3443
11.8	0.3389	0.3407
12.0	0.3354	0.3372
12.2	0.3321	0.3338
12.4	0.3296	0.3304
12.6	0.3281	0.3272
12.8	0.3271	0.3240
13.0	0.3268	0.3210

13.2	0.3264	0.3180
13.4	0.3257	0.3151
13.6	0.3237	0.3123
13.8	0.3200	0.3095
14.0	0.3149	0.3067
14.2	0.3079	0.3039
14.4	0.3008	0.3011
14.6	0.2935	0.2983
14.8	0.2870	0.2955
15.0	0.2822	0.2929
15.2	0.2792	0.2904
15.4	0.2779	0.2880
15.6	0.2775	0.2857
15.8	0.2780	0.2836
16.0	0.2782	0.2815
16.2	0.2782	0.2795
16.4	0.2781	0.2776
16.6	0.2775	0.2758
16.8	0.2772	0.2740
17.0	0.2761	0.2723
17.2	0.2747	0.2706
17.4	0.2733	0.2690
17.6	0.2716	0.2673
17.8	0.2697	0.2657
18.0	0.2675	0.2641
18.2	0.2657	0.2624
18.4	0.2639	0.2608
18.6	0.2615	0.2591
18.8	0.2595	0.2575
19.0	0.2570	0.2559
19.2	0.2541	0.2543
19.4	0.2507	0.2528
19.6	0.2477	0.2513
19.8	0.2452	0.2498
20.0	0.2433	0.2484
20.2	0.2422	0.2471
20.4	0.2415	0.2458
20.6	0.2414	0.2446
20.8	0.2417	0.2435
21.0	0.2421	0.2425
21.2	0.2425	0.2415
21.4	0.2426	0.2406
21.6	0.2423	0.2397
21.8	0.2418	0.2388
22.0	0.2408	0.2380
22.2	0.2399	0.2371
22.4	0.2385	0.2363
22.6	0.2372	0.2355
22.8	0.2357	0.2347
23.0	0.2342	0.2339
23.2	0.2328	0.2331
23.4	0.2317	0.2324

23.6	0.2309	0.2317
23.8	0.2302	0.2310
24.0	0.2296	0.2303
24.2	0.2290	0.2297
24.4	0.2284	0.2291
24.6	0.2277	0.2285
24.8	0.2272	0.2280
25.0	0.2265	0.2274
25.2	0.2263	0.2269
25.4	0.2258	0.2265
25.6	0.2257	0.2260
25.8	0.2254	0.2256
26.0	0.2255	0.2253
26.2	0.2253	0.2250
26.4	0.2253	0.2247
26.6	0.2252	0.2245
26.8	0.2251	0.2244
27.0	0.2250	0.2242
27.2	0.2246	0.2241
27.4	0.2246	0.2241
27.6	0.2240	0.2240
27.8	0.2239	0.2240
28.0	0.2237	0.2240
28.2	0.2237	0.2240
28.4	0.2238	0.2241
28.6	0.2238	0.2243
28.8	0.2242	0.2245
29.0	0.2246	0.2247
29.2	0.2251	0.2250
29.4	0.2258	0.2254
29.6	0.2260	0.2259
29.8	0.2266	0.2263
30.0	0.2270	0.2269
30.2	0.2275	0.2274
30.4	0.2280	0.2281
30.6	0.2287	0.2287
30.8	0.2293	0.2294
31.0	0.2298	0.2301
31.2	0.2305	0.2308
31.4	0.2315	0.2316
31.6	0.2321	0.2324
31.8	0.2329	0.2332
32.0	0.2338	0.2341
32.2	0.2347	0.2350
32.4	0.2361	0.2360
32.6	0.2373	0.2370
32.8	0.2381	0.2380
33.0	0.2392	0.2390

Table S3 Equilibrium distribution of AMP conformers [a]

Method	Conformer	φ_1	φ_2	φ_3	ΔE_e	ΔH	S_{298}	ΔG_{298}	p_{298}
B3LYP/6-31G(d,p) [b]	*gauche-gauche*	62.6	103.8	15.1	0.0	0.3	412.0	1.1	37.9
	gauche-anti	63.5	180.0	0.0	0.1	0.0	414.8	0.0	59.4
	anti-gauche	169.0	-59.2	0.1	6.3	6.2	409.0	7.9	2.4
	anti-anti	167.8	151.5	-1.8	13.2	12.5	411.7	13.4	0.3
B3LYP/cc-pVTZ	*gauche-gauche*	63.4	102.9	12.2	0.6	1.0	408.6	1.3	35.0
	gauche-anti	64.1	180.0	0.0	0.0	0.0	409.6	0.0	59.5
	anti-gauche	167.9	-60.8	-0.1	5.8	5.8	406.9	6.6	4.2
	anti-gauche-2	165.0	101.8	2.0	12.6	12.1	413.2	10.7	0.6
	anti-anti	167.6	160.7	-0.8	11.9	11.2	408.9	11.4	0.7
B3LYP/6-311+G(3df,2p)	*gauche-gauche*	63.7	104.5	0.4	0.4	0.6	410.6	0.0	53.5
	gauche-anti	64.3	180.0	0.0	0.0	0.0	406.3	0.7	40.7
	anti-gauche	167.2	-59.5	0.7	5.3	5.2	405.6	6.1	4.5
	anti-gauche-2	165.4	102.1	1.5	12.1	11.7	409.6	11.4	0.7
	anti-anti	168.2	164.9	-0.7	11.6	10.9	408.6	10.9	0.6
MP2/6-311+G(d,p)	*gauche-gauche*	61.2	90.0	4.0	0.0	0.0	401.6	0.0	50.0
	gauche-anti	61.2	180.0	0.0	2.3	1.9	403.4	1.4	28.6
	anti-gauche	173.9	-55.7	-0.1	3.0	2.7	403.2	2.2	20.3
	anti-gauche-2	174.0	86.2	2.9	11.8	11.3	402.9	10.9	0.6
	anti-anti	175.7	170.2	0.3	14.3	13.1	408.3	11.1	0.5
MP2/6-311+G(2df,p)	*gauche-gauche*	61.1	91.2	6.0	0.0	0.0	403.2	0.0	55.4
	gauche-anti	61.2	180.0	0.0	2.5	2.0	404.9	1.5	30.4
	anti-gauche	175.0	-55.7	0.4	4.6	4.2	405.3	3.6	13.1
	anti-gauche-2	174.1	88.1	3.5	11.4	11.0	403.1	11.0	0.6
	anti-anti	175.5	171.1	-0.5	14.2	13.1	408.4	11.6	0.5
MP2/cc-pVTZ	*gauche-gauche*	60.6	91.2	8.2	0.0	0.0	405.5	0.0	45.0
	gauche-anti	60.8	180.0	0.0	2.6	2.0	411.9	0.1	44.0
	anti-gauche	175.7	-57.0	-1.6	4.9	4.5	407.9	3.8	9.9
	anti-gauche-2	174.4	87.8	2.4	11.2	10.7	405.3	10.8	0.6

	anti-anti	175.2	163.9	0.5	13.8	12.8	411.4	11.0	0.5
MP2/aug-cc-pVTZ [c]	*gauche-gauche*	60.7	91.9	3.4	0.	0.	405.5	0.0	49.1
	gauche-anti	60.8	180.0	0.	3.0	2.4	411.9	0.6	39.0
	anti-gauche	175.9	-55.3	-0.1	4.9	4.5	407.9	3.7	10.8
	anti-gauche-2	175.1	87.9	2.3	11.2	10.7	405.3	10.8	0.6
	anti-anti	176.0	168.2	0.2	14.2	13.1	411.4	11.4	0.5
GED	*gauche-gauche*	61.1 [d]	96.5(45)	6.0 [d]					68 ± 7
	gauche-anti	61.2 [d]	180.0 [d]	0.0 [d]					15 ± 7
	anti-gauche	175.0 [d]	-55.7 [d]	0.4 [d]					17 ± 7

[a] Torsional angles φ_1 = φ(N3–C4–N5–C7), φ_2 = φ(N2-N3-C4-N5), φ_3 = φ(C6-C8-C9-C7) in degrees; ΔE_e (kJ/mol) is the relative electronic energy; $H = E_e$ + ZPE (kJ/mol), where ZPE is the zero point energy correction calculated from scaled vibrational frequencies; S_{298} (J/(K mol)) is the entropy value at 298 K calculated using scaled frequencies and including the entropy of mixing (Rln2) for conformers with C_1 symmetry, which are present as an equimolar mixture of the two optical isomers; $\Delta G_T(i) = \Delta H(i) + T\,\Delta S_T(i)$ is the Gibbs free energy difference (kJ/mol); $p_T(i) = [\exp(-\Delta G_T(i)/RT)]/[\sum_i [\exp(-\Delta G_T(i)/RT)]$ is the mole fraction of conformers (%). [b] *Anti-gauche*-2 conformer was not detected at this level of theory. [c] Values of ZPE and vibrational frequencies from MP2/cc-pVTZ calculation are used. [d] Assumed at the value from MP2/6-311+G(2df,p) calculation.

Table S4 Molecular structure of *gauche-anti* conformer of AMP obtained by gas-phase electron diffraction and quantum chemical calculations

Parameter [a]	GED single conformer model $r_{h1}(\angle_{h1})$ [b]	GED mixture of conformers $r_{h1}(\angle_{h1})$ [b]	B3LYP /cc-pVTZ $r_e(\angle_e)$	MP2 /6-311+G(2df,p) $r_e(\angle_e)$
Independent parameters				
r(N1–N2)	1.154(4)	1.158(2)	1.134	1.153
r(N2–N3)	1.218(5)	1.231(2)	1.221	1.228
r(C4–N3)	1.497(4)	1.505(10)	1.524	1.515
r(C4–N5)	1.389(7)	1.394(8)	1.411	1.413
r(C6–N5) = r(C7–N5)	1.472(4)	1.478(7)	1.463	1.461
r(C6–C8) = r(C7–C9)	1.539(4) [1]	1.543(3) [1]	1.536	1.529
r(C8–C9)	1.559(4) [1]	1.563(3) [1]	1.554	1.549
$r(C–H)_{av}$	1.094(8) [c]	1.099(4) [c]	1.092	1.094
∠N1–N2–N3	175.6 [d]	175.6 [d]	176.2	175.6
∠C4–N3–N2	117.7(7) [2]	116.6(5) [2]	114.7	114.0
∠N3–C4–N5	114.7(7) [2]	113.0(5) [2]	112.0	111.0
∠C4–N5–C6 = ∠C4–N5–C7	119.3(7) [2]	116.7(5) [2]	117.3	115.6
∠C6–C8–C9 = ∠C7–C9–C8	104.4(7)	104.4 [d]	104.8	104.4
φ(N5–C6–C7–C9)	141.5(26)	134.7 [d]	138.9	134.7
φ(N1–N2–N3–C4)	180	180	180	180
$φ_2$(N2–N3–C4–N5)	180	180	180	180
mole fraction:				
gauche-gauche		68(7)		
gauche-anti	100	15(7)		
anti-gauche		17(7)		
Dependent parameters				
∠N5–C6–C8 = ∠N5–C7–C9	105.5(20)	102.9(5)	103.5	102.8
∠C6–N5–C7	104.4(17)	104.0(9)	106.2	104.4
$φ_1$(N3–C4–N5–C7) = -φ(N3–C4–N5–C6)	64.9(26)	61.8(17)	64.1	61.2

φ(C7–N5–C6–C8) = φ(C6–N5–C7–C9)	-38.7(27)	-44.9(5)	-40.8	-44.9
φ(N5–C6–C8–C9) = φ(N5–C7–C9–C8)	23.3(18)	26.7(3)	24.0	26.5
φ_3(C6–C8–C9–C7)	0	0	0	0
R_L	8.5	1.5		
R_S	9.9	6.4		
R_{tot}	9.1	4.2		

[a] Bond lengths are in Å, bond angles and torsional angles (φ) are in degrees, mole fraction in %. Together with total value of the disagreement factor (R_{tot}), the *R* factors (in %) are given for long (R_L) and short (R_S) camera distances. [b] Values in parentheses are three times the standard deviations. The same numeric superscripts indicate that these parameters were refined in one group; differences between parameters in the group were assumed at the values from MP2/6-311+G(2df,p) calculation. [c] All C–H bond lengths were refined in one group; their average value is given in the Table. [d] Assumed at the value from MP2/6-311+G(2df,p) calculation.

TABLE S5 Molecular structure of *anti-gauche* conformer of AMP obtained by gas-phase electron diffraction and quantum chemical calculations

Parameter [a]	GED single conformer model $r_{h1}(\angle_{h1})$ [b]	GED mixture of conformers $r_{h1}(\angle_{h1})$ [b]	B3LYP /cc-pVTZ $r_e(\angle_e)$	MP2 /6-311+G(2df,p) $r_e(\angle_e)$
independent parameters				
r(N1–N2)	1.157(5)	1.154(2)	1.129	1.149
r(N2–N3)	1.240(5)	1.239(2)	1.229	1.236
r(C4–N3)	1.466(7) [1]	1.463(10)	1.477	1.472
r(C4–N5)	1.433(7) [1]	1.420(8)	1.441	1.438
r(C6–N5)	1.490(6) [2]	1.478(7) [1]	1.464	1.461
r(C7–N5)	1.490(6) [2]	1.478(7) [1]	1.464	1.461
r(C6–C8)	1.543(7) [3]	1.542(3) [2]	1.536	1.529
r(C7–C9)	1.543(7) [3]	1.543(3) [2]	1.535	1.529
r(C8–C9)	1.562(7) [3]	1.561(3) [2]	1.553	1.548
r(C–H)$_{av}$	1.113(7) [c]	1.110(4) [c]	1.093	1.095
∠N1–N2–N3	173.4 [d]	173.4 [d]	173.6	173.4
∠C4–N3–N2	114.7(6) [4]	115.5(6) [3]	115.0	113.5
∠N3–C4–N5	112.6(6) [4]	113.4(6) [3]	112.6	111.4
∠C4–N5–C6	113.8 (6) [4]	113.7(5) [4]	114.3	112.6
∠C4–N5–C7	114.9(6) [4]	114.8(5) [4]	115.4	113.7
∠N5–C6–C8	103.1(16)	103.0 [d]	103.6	103.0
φ(N1–N2–N3–C4)	177.2 [d]	177.2 [d]	179.6	177.2
φ_2(N2–N3–C4–N5)	-55.7 [d]	-55.7 [d]	-60.8	-55.7
φ(N3–C4–N5–C6)	-67.4 [d]	-67.4 [d]	-70.0	-67.4
φ_1(N3–C4–N5–C7)	175.0 [d]	175.0 [d]	167.9	175.0
φ(C7–N5–C6–C8)	-45.5 [d]	-45.5 [d]	-42.1	-45.5
φ(C6–C8–C7–C9)	179.6 [d]	179.6 [d]	179.9	179.6
mole fraction:				
gauche-gauche		68(7)		
gauche-anti		15(7)		
anti-gauche	100	17(7)		
dependent parameters				
∠N5–C7–C9	103.4(13)	104.0(10)	103.6	103.0
∠C6–C8–C9	104.6(20)	104.9(7)	104.6	104.2
∠C7–C9–C8	103.9(16)	103.1(12)	104.6	104.3
∠C6–N5–C7	102.4(8)	102.6(8)	105.2	103.8
φ(C6–N5–C7–C9)	45.9(5)	46.3(3)	42.2	45.3
φ(N5–C6–C8–C9)	27.3(3)	27.2(5)	24.8	27.3
φ(N5–C7–C9–C8)	-27.9(3)	-27.9(3)	-25.0	-26.7
φ_3(C6–C8–C9–C7)	-0.4(2)	-0.4(2)	-0.1	0.4
R_L	9.7	1.5		
R_S	9.6	6.4		
R_{tot}	9.6	4.2		

[a] Bond lengths are in Å, bond angles and torsional angles (φ) are in degrees, mole fraction in %. Together with total value of the disagreement factor (R_{tot}), the R factors (in %) are given for long

(R_L) and short (R_S) camera distances. [b] Values in parentheses are three times the standard deviations. The same numeric superscripts indicate that these parameters were refined in one group; differences between parameters in the group were assumed at the values from MP2/6-311+G(2df,p) calculation. [c] All C–H bond lengths were refined in one group; their average value is given in the Table. [d] Assumed at the value from MP2/6-311+G(2df,p) calculation.

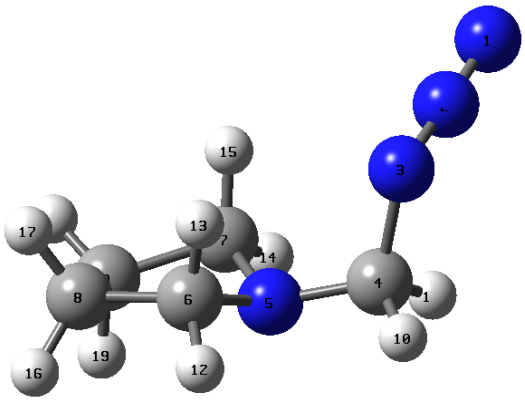
Table S6 Vibrational amplitudes and vibrational corrections for non-hydrogen distances of *gauche-gauche* conformer calculated at different levels of theory [a]

		B3LYP/cc-pVTZ		MP2/cc-pVTZ		MP2/6-311+G(2df,p)[b]	
Distance	r_a	u	$r_{h1} - r_a$	u	$r_{h1} - r_a$	u	$r_{h1} - r_a$
N1–N2	1.146	0.034	0.0010	0.034	0.0004	0.034	0.0004
N2–N3	1.234	0.039	-0.0032	0.038	-0.0022	0.038	-0.0022
C4–N5	1.413	0.049	-0.0029	0.049	-0.0017	0.049	-0.0017
N5–C6	1.468	0.050	-0.0053	0.050	-0.0053	0.049	-0.0038
N5–C7	1.472	0.051	-0.0005	0.050	-0.0025	0.050	-0.0023
N3–C4	1.507	0.059	0.0064	0.057	0.0050	0.057	0.0050
C6–C8	1.536	0.053	-0.0032	0.053	-0.0009	0.053	0.0001
C7–C9	1.546	0.054	0.0072	0.054	0.0051	0.054	0.0035
C8–C9	1.552	0.054	0.0051	0.053	0.0066	0.053	0.0055
N2···C4	2.328	0.068	-0.0028	0.070	-0.0058	0.070	-0.0048
N5···C8	2.328	0.070	0.0098	0.077	0.0151	0.075	0.0140
C6···C7	2.356	0.074	0.0099	0.069	0.0047	0.065	0.0030
N5···C9	2.360	0.077	0.0352	0.086	0.0296	0.080	0.0219
N1···N3	2.370	0.043	0.0065	0.044	0.0061	0.044	0.0059
C6···C9	2.408	0.081	0.0277	0.083	0.0347	0.077	0.0289
C7···C8	2.435	0.072	0.0451	0.075	0.0452	0.072	0.0346
C4···C7	2.453	0.069	-0.0068	0.069	-0.0078	0.069	-0.0059
N3···N5	2.459	0.071	-0.0004	0.067	0.0018	0.067	0.0016
C4···C6	2.463	0.070	-0.0099	0.069	-0.0099	0.069	-0.0073
N3···C7	3.037	0.137	-0.0068	0.128	-0.0048	0.129	-0.0028
N3···C6	3.087	0.144	-0.0129	0.132	-0.0136	0.130	-0.0111
N2···N5	3.188	0.170	0.0445	0.121	0.0096	0.120	0.0112
N2···C6	3.337	0.297	0.0466	0.192	-0.0090	0.192	-0.0039
N1···C4	3.382	0.092	-0.0362	0.098	-0.0265	0.098	-0.0249
C4···C8	3.668	0.072	0.0090	0.074	0.0138	0.073	0.0139
C4···C9	3.674	0.075	0.0416	0.076	0.0363	0.074	0.0269
N2···C7	3.963	0.215	0.0810	0.171	0.0302	0.170	0.0324
N1···C6	3.994	0.463	0.0661	0.294	-0.0254	0.291	-0.0188
N1···N5	4.151	0.251	0.0395	0.181	-0.0059	0.178	-0.0031
N3···C9	4.261	0.179	0.0368	0.158	0.0396	0.145	0.0298
N3···C8	4.346	0.138	0.0087	0.126	0.0124	0.126	0.0119
N2···C8	4.742	0.302	0.0755	0.193	0.0160	0.193	0.0203
N2···C9	4.956	0.295	0.1338	0.239	0.0795	0.221	0.0693
N1···C7	4.969	0.306	0.1273	0.232	0.0479	0.229	0.0503
N1···C8	5.408	0.499	0.1132	0.318	0.0035	0.314	0.0113
N1···C9	5.800	0.448	0.1970	0.346	0.1007	0.324	0.0904

[a] Values of distances (r_a), amplitudes (u), and vibrational corrections (r_{h1}–r_a) are in Å**.** The amplitudes and vibrational corrections for which the B3LYP calculation gives the overestimated values are underlined. [b] These amplitudes and vibrational corrections were used in GED analysis.

Table S7 Vibrational amplitudes (u) and harmonic ($r_{h1} - r_a$) vibrational corrections (in Å) obtained from the MP2/6-311+G(2df,p) force field for different conformers of AMP

Distance		r_a	u	$r_{h1} - r_a$
		gauche-gauche **conformer**		
C4	H10	1.106480	0.075900	0.001050
C9	H18	1.106827	0.076200	0.001370
C8	H17	1.106955	0.076100	0.001410
C9	H19	1.107077	0.076200	0.001390
C8	H16	1.107579	0.076200	0.001330
C7	H14	1.109126	0.076300	0.001310
C6	H12	1.109325	0.076400	0.001360
C4	H11	1.109630	0.076600	0.001480
C7	H15	1.115852	0.077700	0.001050
C6	H13	1.119122	0.077900	0.000960
N1	N2	1.146843	0.033900	0.000390
N2	N3	1.230807	0.038100	-0.002170
C4	N5	1.401422	0.048500	-0.001660
N5	C6	1.475032	0.049300	-0.003780
N5	C7	1.479009	0.049500	-0.002300
N3	C4	1.504468	0.056800	0.005010
C6	C8	1.533784	0.052600	0.000080
C7	C9	1.544224	0.053600	0.003460
C8	C9	1.549611	0.052500	0.005460
H18	H19	1.778637	0.122500	0.005200
H16	H17	1.785611	0.122800	0.005530
H14	H15	1.793694	0.122200	0.005340
H12	H13	1.798551	0.122400	0.005610
H10	H11	1.798836	0.122300	0.010270
N5	H11	1.990577	0.101300	0.005680
N3	H10	2.072518	0.105600	0.010610
N5	H10	2.105672	0.100600	0.005300
N5	H14	2.129739	0.103500	-0.000290
N5	H12	2.133558	0.103300	-0.001700
N3	H11	2.134469	0.104000	0.006280
N5	H15	2.147099	0.102000	0.002080
N5	H13	2.154814	0.102600	0.001660
C6	H16	2.169703	0.112100	0.004330
C8	H13	2.188466	0.106400	0.007350
C9	H16	2.193208	0.106700	0.009670
C7	H19	2.193329	0.107600	0.004170
C9	H15	2.198464	0.106500	0.008160
C7	H18	2.203617	0.116500	0.005480
C6	H17	2.204589	0.107900	0.002080
C8	H18	2.204622	0.107400	0.007910
C8	H19	2.209945	0.110700	0.006420
C8	H12	2.215752	0.106100	0.001550
C9	H14	2.218945	0.106300	0.004100
C9	H17	2.220937	0.106400	0.006420
N5	C8	2.334353	0.074500	0.013960
N2	C4	2.335414	0.070300	-0.004750
C6	C7	2.350641	0.065300	0.002970
H15	H19	2.365416	0.211200	-0.019570
N1	N3	2.367896	0.043700	0.005890
N5	C9	2.373728	0.080200	0.021910
H16	H18	2.406176	0.191600	-0.046190
C6	C9	2.410077	0.076900	0.028920
H14	H18	2.419848	0.181500	-0.032270
C7	C8	2.425558	0.071700	0.034550
H12	H16	2.433680	0.179000	-0.016510

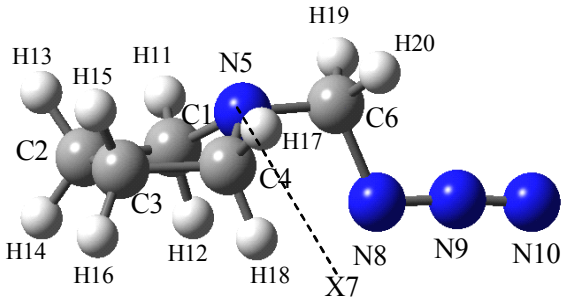


H13	H17	2.434190	0.206500	-0.001220
H17	H19	2.442933	0.186500	-0.044510
N3	N5	2.459428	0.067000	0.001630
N2	H11	2.466123	0.156300	-0.026420
C4	C7	2.468499	0.068800	-0.005930
C4	C6	2.477566	0.068700	-0.007320
H11	H12	2.479229	0.215900	-0.016080
C6	H11	2.617337	0.150300	0.000650
C4	H15	2.725536	0.171100	-0.004780
H10	H14	2.727389	0.221700	-0.025030
N5	H16	2.753764	0.283700	0.052760
C7	H13	2.758886	0.148900	0.006450
H12	H17	2.763091	0.179000	0.001340
N3	H15	2.764010	0.234800	-0.023320
C7	H10	2.789927	0.150300	-0.001780
H13	H15	2.800230	0.267800	0.001910
C4	H12	2.800513	0.139600	-0.012080
C4	H13	2.804426	0.153600	-0.003750
C6	H15	2.820553	0.191700	0.013070
C4	H14	2.832221	0.148500	-0.011630
H17	H18	2.850999	0.207200	0.035580
C9	H13	2.863672	0.241300	0.057010
N2	H13	2.869667	0.254100	-0.006990
H14	H19	2.876141	0.200400	0.011110
N3	H13	2.885937	0.227700	-0.021430
H15	H18	2.984287	0.146700	0.037600
H16	H19	2.987578	0.181800	0.040920
N5	H18	2.994429	0.325000	0.074040
H11	H13	3.016606	0.221400	0.011160
C7	H16	3.018989	0.239500	0.083350
C6	H19	3.025369	0.290500	0.084430
H13	H16	3.048283	0.132800	0.030200
C8	H15	3.054627	0.253400	0.069050
H10	H15	3.056055	0.267300	0.013530
H13	H19	3.074545	0.567400	0.161460
N3	C7	3.078911	0.128600	-0.002790
N2	H10	3.079435	0.110600	0.007120
N3	C6	3.128107	0.130400	-0.011120
N2	N5	3.180047	0.120300	0.011150
N5	H19	3.180659	0.145900	0.059850
C6	H18	3.214693	0.209500	0.074910
C7	H17	3.247151	0.228800	0.079310
C8	H14	3.253309	0.149700	0.066150
N5	H17	3.272676	0.112800	0.040100
C6	H14	3.284183	0.098600	0.017270
N1	H11	3.289395	0.214300	-0.073790
C7	H12	3.316946	0.098300	0.010350
N1	H13	3.343282	0.353300	0.004590
C7	H11	3.351665	0.100200	0.007490
C9	H12	3.353890	0.112700	0.048060
N2	C6	3.364497	0.191500	-0.003850
N1	C4	3.393121	0.097700	-0.024900
C6	H10	3.433240	0.100200	0.005450
H14	H16	3.567998	0.443600	0.147590
N3	H12	3.574538	0.197000	-0.010130
N3	H14	3.579063	0.225100	0.009000
N2	H12	3.580520	0.284600	-0.020840
H15	H17	3.595099	0.529400	0.155930
N2	H15	3.648122	0.271400	0.026470
C4	C8	3.671052	0.073100	0.013900
C4	C9	3.687264	0.073600	0.026910
H11	H15	3.719683	0.172500	0.009580
H11	H14	3.750713	0.161900	0.002420

H10	H12	3.762994	0.157500	0.004020
H13	H14	3.805292	0.164400	0.023860
H10	H13	3.840925	0.168400	0.007680
H13	H18	3.844733	0.181300	0.101890
H12	H15	3.856533	0.187300	0.017360
H15	H16	3.862933	0.181600	0.112750
C8	H11	3.959185	0.148400	0.015610
N2	C7	3.981868	0.170100	0.032430
H12	H18	3.982551	0.355600	0.115460
N1	C6	4.012340	0.290500	-0.018830
H12	H19	4.033403	0.256000	0.108320
N1	H12	4.060749	0.386000	-0.064350
C4	H16	4.072433	0.281900	0.046470
H12	H14	4.125594	0.136200	0.019940
H14	H17	4.136774	0.192000	0.121740
N1	N5	4.141038	0.177800	-0.003100
N1	H10	4.160874	0.132100	-0.002030
C9	H10	4.169762	0.152900	0.030060
H11	H16	4.201303	0.310800	0.029380
C4	H18	4.299907	0.324300	0.077320
N3	C9	4.323364	0.144700	0.029790
C9	H11	4.333511	0.127300	0.043200
C4	H19	4.369255	0.208600	0.075660
N3	C8	4.396525	0.125800	0.011930
C8	H10	4.419928	0.123400	0.030960
C4	H17	4.523664	0.142100	0.042200
H10	H18	4.605331	0.375600	0.067040
N1	H15	4.607186	0.330600	0.066360
N2	H14	4.641157	0.217100	0.041400
N3	H19	4.687997	0.394300	0.083490
H10	H16	4.705064	0.359500	0.074340
H11	H17	4.774094	0.176200	0.038790
N2	C8	4.779010	0.192600	0.020250
H10	H19	4.888180	0.194400	0.071390
H11	H18	4.899648	0.416300	0.106510
N1	C7	4.977047	0.229100	0.050270
N2	C9	4.998156	0.220600	0.069320
N3	H17	5.022338	0.280800	0.036450
N3	H16	5.059141	0.201900	0.048150
H11	H19	5.081173	0.223700	0.102480
N3	H18	5.133012	0.200900	0.079520
N2	H17	5.243568	0.300800	0.030570
N2	H19	5.274323	0.526600	0.154270
H10	H17	5.349182	0.168300	0.069140
N1	C8	5.436293	0.313500	0.011250
N2	H16	5.470834	0.229800	0.038060
N1	H14	5.711586	0.234400	0.060910
N1	H17	5.742546	0.408800	0.017500
N1	C9	5.831073	0.323900	0.090440
N2	H18	5.890825	0.212800	0.122110
N1	H19	6.016964	0.648200	0.203790
N1	H16	6.142668	0.326900	0.006480
N1	H18	6.768680	0.281000	0.141990

gauche-anti **conformer**

C2	H14	1.106853	0.076200	0.001420
C3	H16	1.106853	0.076300	0.001420
C3	H15	1.107134	0.076400	0.001370
C2	H13	1.107144	0.076300	0.001360
C4	H17	1.109119	0.076300	0.001320
C1	H11	1.109119	0.076300	0.001320
C6	H19	1.110661	0.076700	0.001380
C6	H20	1.110661	0.076700	0.001380

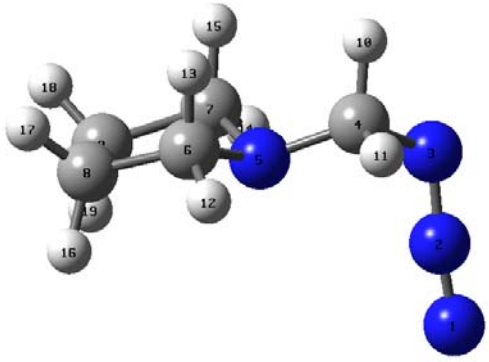


C4	H18	1.116929	0.077600	0.001000
C1	H12	1.116929	0.077600	0.001000
N10	N9	1.147298	0.033800	0.000490
N9	N8	1.228776	0.037700	-0.001860
C6	N5	1.395612	0.047400	-0.002290
N5	C1	1.479361	0.049500	-0.005010
N5	C4	1.479361	0.049500	-0.005010
N8	C6	1.506911	0.057000	0.005390
C1	C2	1.537657	0.054900	0.002500
C4	C3	1.537657	0.054900	0.002500
C2	C3	1.550357	0.052200	0.007790
H15	H16	1.782619	0.122800	0.003860
H13	H14	1.782629	0.122800	0.003850
H11	H12	1.796958	0.122200	0.004720
H17	H18	1.796958	0.122200	0.004720
H19	H20	1.804043	0.122100	0.008910
N5	H19	2.047597	0.101000	0.006450
N5	H20	2.047597	0.101000	0.006450
N8	H20	2.129014	0.104800	0.005510
N8	H19	2.129014	0.104800	0.005510
N5	H17	2.136299	0.103400	-0.004440
N5	H11	2.136299	0.103400	-0.004440
N5	H12	2.147816	0.102000	-0.000240
N5	H18	2.147816	0.102000	-0.000240
C1	H13	2.186158	0.120700	0.004370
C4	H15	2.186158	0.120700	0.004370
C3	H13	2.194361	0.107700	0.009250
C2	H15	2.194361	0.107800	0.009250
C4	H16	2.198973	0.107400	0.001750
C1	H14	2.198973	0.107300	0.001750
C2	H12	2.203203	0.107000	0.008500
C3	H18	2.203203	0.107000	0.008500
C3	H17	2.214924	0.106500	0.001470
C2	H11	2.214924	0.106500	0.001470
C3	H14	2.222361	0.108300	0.006150
C2	H16	2.222361	0.108400	0.006150
N9	C6	2.328943	0.073000	-0.010680
N5	C2	2.341638	0.085700	0.023870
N5	C3	2.341648	0.085700	0.023860
C1	C4	2.352799	0.062800	0.002530
N10	N8	2.366772	0.043300	0.006660
H13	H15	2.398981	0.187800	-0.071140
N8	N5	2.410825	0.065000	0.006680
C4	C2	2.414014	0.075800	0.044040
C1	C3	2.414014	0.075800	0.044040
H18	H16	2.419406	0.220800	-0.017160
H12	H14	2.419416	0.220800	-0.017170
H17	H15	2.430254	0.180000	-0.037980
H11	H13	2.430264	0.180000	-0.037990
H14	H16	2.465359	0.186700	-0.066360
C6	C4	2.466971	0.067900	-0.010690
C6	C1	2.466971	0.067900	-0.010690
H19	H11	2.597747	0.218600	-0.028940
H20	H17	2.597757	0.218600	-0.028950
N9	H19	2.627497	0.224000	-0.022110
N9	H20	2.627497	0.224000	-0.022110
C4	H20	2.700625	0.151200	-0.002940
C1	H19	2.700625	0.151200	-0.002940
N8	H12	2.736134	0.227900	-0.022930
N8	H18	2.736144	0.227900	-0.022940
C6	H18	2.754198	0.167300	-0.009010
C6	H12	2.754198	0.167200	-0.009010
H12	H18	2.775169	0.240000	-0.012450

C4	H12	2.777447	0.168200	0.007670
C1	H18	2.777447	0.168200	0.007670
H11	H14	2.810087	0.207400	0.004100
H17	H16	2.810087	0.207400	0.004100
C6	H17	2.811449	0.144300	-0.019830
C6	H11	2.811449	0.144300	-0.019830
N5	H13	2.837012	0.360600	0.086140
N5	H15	2.837022	0.360600	0.086130
H14	H15	2.914921	0.213400	0.047510
H13	H16	2.914921	0.213500	0.047510
C3	H12	2.947649	0.280500	0.084900
C2	H18	2.947649	0.280500	0.084900
H12	H13	3.028145	0.139000	0.040480
H18	H15	3.028145	0.138900	0.040480
H20	H18	3.032235	0.255200	0.010550
H19	H12	3.032235	0.255200	0.010550
N8	C1	3.032431	0.125600	-0.003910
N8	C4	3.032431	0.125600	-0.003910
C4	H13	3.099447	0.257600	0.106990
C1	H15	3.099447	0.257600	0.106990
C1	H16	3.129864	0.294200	0.109520
C4	H14	3.129864	0.294200	0.109520
N5	H14	3.221434	0.131000	0.063310
N5	H16	3.221444	0.130900	0.063300
C2	H17	3.300054	0.134000	0.075030
C3	H11	3.300054	0.134000	0.075030
H12	H16	3.305257	0.638200	0.215900
H18	H14	3.305267	0.638200	0.215890
C1	H17	3.307855	0.098700	0.012770
C4	H11	3.307855	0.098700	0.012770
N10	C6	3.388315	0.104700	-0.043990
C4	H19	3.394317	0.099900	0.003860
C1	H20	3.394317	0.099900	0.003860
N9	N5	3.472987	0.072800	0.040820
N8	H11	3.519755	0.214700	-0.000900
N8	H17	3.519755	0.214700	-0.000900
N10	H20	3.520668	0.318200	-0.073780
N10	H19	3.520748	0.317800	-0.073860
C6	C3	3.662793	0.076500	0.024800
C6	C2	3.662793	0.076600	0.024800
N9	H12	3.745202	0.301300	0.068410
N9	H18	3.745212	0.301200	0.068400
H17	H13	3.748468	0.462300	0.176090
H11	H15	3.748478	0.462200	0.176080
H19	H17	3.763536	0.159100	-0.003610
H20	H11	3.763536	0.159100	-0.003610
H19	H18	3.772837	0.172100	0.004360
H20	H12	3.772837	0.172100	0.004360
H11	H18	3.820568	0.169900	0.017850
H12	H17	3.820568	0.169900	0.017850
H12	H15	3.839378	0.181300	0.141530
H18	H13	3.839378	0.181300	0.141530
C3	H20	4.049902	0.156200	0.027040
C2	H19	4.049902	0.156200	0.027040
H17	H14	4.078463	0.235700	0.151750
H11	H16	4.078483	0.235500	0.151730
N9	C1	4.096818	0.187800	0.062200
N9	C4	4.096818	0.187800	0.062200
H11	H17	4.143239	0.134800	0.014770
C6	H13	4.146965	0.356800	0.079970
C6	H15	4.146985	0.356700	0.079950
N8	C3	4.281315	0.130300	0.032240
N8	C2	4.281315	0.130400	0.032240

H19	H13	4.363557	0.394200	0.060800
H20	H15	4.363577	0.394100	0.060780
C2	H20	4.364736	0.129900	0.045060
C3	H19	4.364736	0.129800	0.045060
N9	H11	4.428792	0.317300	0.047850
N9	H17	4.428792	0.317300	0.047850
C6	H14	4.438746	0.184300	0.072890
C6	H16	4.438776	0.184000	0.072860
N10	N5	4.575407	0.094800	0.043610
N10	H12	4.755648	0.375800	0.135470
N10	H18	4.755678	0.375600	0.135440
H20	H13	4.761423	0.450800	0.116610
H19	H15	4.761443	0.450700	0.116590
N8	H14	4.776337	0.373600	0.083230
N8	H16	4.776357	0.373400	0.083210
H19	H14	4.825450	0.184200	0.066970
H20	H16	4.825470	0.183900	0.066950
N8	H13	5.014704	0.217800	0.085270
N8	H15	5.014734	0.217500	0.085240
N10	C4	5.163013	0.258300	0.101220
N10	C1	5.163013	0.258200	0.101220
H20	H14	5.211979	0.204700	0.106390
H19	H16	5.212009	0.204400	0.106360
N9	C2	5.400204	0.154800	0.111830
N9	C3	5.400214	0.154700	0.111820
N10	H17	5.409889	0.437100	0.077530
N10	H11	5.409909	0.437000	0.077510
N9	H14	5.877591	0.397700	0.177730
N9	H16	5.877621	0.397500	0.177700
N9	H13	6.094580	0.253000	0.154620
N9	H15	6.094620	0.252500	0.154580
N10	C3	6.481557	0.194600	0.166910
N10	C2	6.481557	0.194800	0.166910
N10	H14	6.922529	0.437900	0.256930
N10	H16	6.922569	0.437500	0.256890
N10	H13	7.164203	0.295500	0.197210
N10	H15	7.164243	0.295000	0.197170

***anti-gauche* conformer**



C7	H14	1.106710	0.076100	0.001350
C9	H19	1.106977	0.076100	0.001330
C9	H18	1.107002	0.076100	0.001420
C8	H16	1.107003	0.076100	0.001330
C8	H17	1.107020	0.076100	0.001410
C6	H12	1.108607	0.076300	0.001340
C4	H11	1.111755	0.076900	0.001240
C4	H10	1.116846	0.077500	0.000790
C6	H13	1.121807	0.078300	0.001090
C7	H15	1.121852	0.078300	0.001110
N1	N2	1.142482	0.033700	0.000270
N2	N3	1.237190	0.038400	-0.001870
C4	N5	1.423641	0.048200	-0.000310
N3	C4	1.463023	0.051300	0.002610
N5	C6	1.477236	0.049500	-0.002790
N5	C7	1.477877	0.049600	-0.002780
C7	C9	1.537125	0.053200	0.001930
C6	C8	1.538748	0.053100	0.001410
C8	C9	1.552390	0.052100	0.004860
H18	H19	1.780351	0.122500	0.005960
H16	H17	1.781300	0.122400	0.005960
H14	H15	1.793895	0.122500	0.005950
H12	H13	1.797073	0.122500	0.005980
H10	H11	1.798714	0.122400	0.008450

N3	H10	2.043804	0.103700	0.006810
N5	H11	2.057890	0.101900	0.005330
N3	H11	2.117151	0.102900	0.005290
N5	H10	2.117924	0.101000	0.005320
N5	H12	2.135701	0.103300	-0.000110
N5	H14	2.137595	0.102900	-0.000440
N5	H15	2.144217	0.102300	0.003150
N5	H13	2.152233	0.102100	0.003280
C6	H16	2.182766	0.115100	0.005520
C7	H19	2.183147	0.115000	0.006260
C8	H13	2.193820	0.107000	0.007080
C7	H18	2.195710	0.107400	0.004550
C6	H17	2.197432	0.107300	0.004000
C9	H16	2.198056	0.107200	0.008420
C9	H15	2.198189	0.107500	0.007450
C8	H19	2.199364	0.106700	0.008710
C9	H14	2.215217	0.106000	0.003640
C8	H12	2.217740	0.106100	0.002840
C9	H17	2.221942	0.107500	0.006450
C8	H18	2.222296	0.108100	0.006800
N2	C4	2.290229	0.065500	-0.002010
C6	C7	2.330021	0.062300	0.002460
N5	C8	2.356934	0.076600	0.014530
N5	C9	2.357584	0.077500	0.015930
N1	N3	2.368363	0.044000	0.006000
H16	H19	2.381693	0.185800	-0.041870
H13	H17	2.394082	0.205500	-0.005770
H15	H18	2.404308	0.205900	-0.007290
N3	N5	2.406377	0.064900	0.004460
H12	H16	2.420065	0.177300	-0.018900
C7	C8	2.420210	0.071200	0.027360
H14	H19	2.423435	0.178000	-0.018710
C6	C9	2.425135	0.071300	0.027350
H17	H18	2.439180	0.185500	-0.038350
C4	C6	2.446104	0.073100	-0.004180
H10	H15	2.459033	0.240800	-0.017350
C4	C7	2.461268	0.069100	-0.004650
H11	H12	2.508712	0.210400	-0.023970
C6	H11	2.584625	0.149000	-0.006140
N2	H11	2.621300	0.172500	-0.004450
H10	H13	2.667441	0.268900	0.007310
H13	H15	2.679674	0.236800	0.000480
C4	H13	2.689668	0.169000	0.000730
C4	H15	2.694894	0.164100	-0.001160
C7	H10	2.697892	0.153600	-0.005840
C6	H15	2.727079	0.162600	0.009740
C7	H13	2.735974	0.156100	0.008930
H14	H18	2.794860	0.185800	0.008010
H12	H17	2.800900	0.185000	0.006730
H11	H13	2.805482	0.244800	0.006480
C4	H12	2.806733	0.140300	-0.007390
C4	H14	2.828521	0.140700	-0.007890
N2	N5	2.841024	0.154900	0.000180
C6	H10	2.858958	0.168600	0.009020
N5	H19	2.862117	0.294200	0.059580
N5	H16	2.863087	0.291300	0.055600
N3	H14	2.865296	0.202900	-0.010990
H16	H18	2.932268	0.184400	0.035620
H17	H19	2.932931	0.189600	0.035550
C8	H15	2.945623	0.236500	0.055850
C9	H13	2.953692	0.231400	0.054170
H13	H16	3.032942	0.135200	0.030530
H15	H19	3.038105	0.136200	0.032480

N3	C7	3.047284	0.133700	0.008760
C7	H16	3.128804	0.217600	0.070120
H10	H14	3.130971	0.223800	-0.002160
C6	H19	3.132393	0.214300	0.071380
N2	H10	3.142074	0.100400	0.019530
C7	H17	3.157570	0.239700	0.071280
C6	H18	3.161872	0.243900	0.072590
N2	H14	3.219501	0.370400	0.051360
N5	H18	3.250164	0.123700	0.046120
N5	H17	3.251429	0.120300	0.042790
C6	H14	3.298917	0.096900	0.012000
C7	H12	3.299027	0.097400	0.011420
C8	H14	3.329163	0.123700	0.049320
C9	H12	3.333175	0.121500	0.048140
H15	H17	3.345352	0.512400	0.138210
N1	C4	3.349658	0.090500	-0.014920
H13	H18	3.353136	0.509900	0.137370
N3	H15	3.362841	0.258100	0.032100
C7	H11	3.377359	0.101400	0.007430
H10	H12	3.384776	0.215600	0.016150
N1	H11	3.518574	0.234300	-0.026610
N2	C7	3.564540	0.268200	0.042930
H11	H15	3.645380	0.175700	0.009660
C4	C8	3.677828	0.071300	0.017910
N1	N5	3.682714	0.233200	-0.023050
C4	C9	3.684208	0.070900	0.019360
N3	C6	3.731135	0.071000	0.009020
H12	H15	3.776110	0.168500	0.018590
H13	H14	3.782568	0.165200	0.019130
H14	H16	3.826895	0.375300	0.114190
H12	H19	3.828490	0.367400	0.113440
H11	H14	3.833900	0.153900	0.008780
H15	H16	3.861272	0.178100	0.095310
H13	H19	3.866416	0.177700	0.096020
N1	H14	3.887187	0.528300	0.103220
C9	H10	4.007841	0.153700	0.021040
C8	H11	4.010521	0.144000	0.013670
N3	H12	4.054564	0.150000	0.003060
C8	H10	4.079341	0.161700	0.028050
N3	H13	4.097367	0.168600	0.019440
H14	H17	4.125633	0.209200	0.100930
H12	H18	4.130870	0.213700	0.100760
N2	C6	4.144256	0.149400	0.000900
H12	H14	4.155303	0.133200	0.016540
N2	H15	4.163834	0.307800	0.071100
C4	H16	4.201952	0.275900	0.054020
C4	H19	4.207630	0.279800	0.058770
N1	H10	4.256364	0.108900	0.022610
N2	H12	4.275403	0.232700	-0.016770
N1	C7	4.358301	0.393400	0.059420
C9	H11	4.373459	0.121200	0.032590
H11	H16	4.403263	0.299300	0.034030
N3	C9	4.410783	0.126000	0.026560
C4	H17	4.447126	0.172800	0.050960
C4	H18	4.452666	0.177800	0.054980
H10	H18	4.556166	0.309700	0.052340
H10	H17	4.650786	0.323500	0.063730
N3	H19	4.696700	0.320500	0.044650
N2	C9	4.709943	0.289900	0.045540
H10	H19	4.713585	0.219600	0.059860
H11	H17	4.736211	0.187700	0.038060
N3	C8	4.736552	0.097000	0.037030
N2	H19	4.742694	0.495300	0.059780

N2	H13	4.751651	0.161500	0.023750
H10	H16	4.805417	0.225800	0.067540
H11	H19	4.868566	0.352600	0.084060
N1	H12	4.899041	0.331800	-0.060370
N1	C6	4.899529	0.246900	-0.028820
N2	C8	5.004828	0.237400	0.034580
N1	H15	5.092962	0.385400	0.094450
N1	H19	5.125055	0.684300	0.068070
N3	H16	5.127053	0.376000	0.081700
N2	H16	5.146999	0.518600	0.071950
H11	H18	5.190154	0.209200	0.077950
N3	H18	5.192278	0.169500	0.060950
N1	C9	5.305632	0.464600	0.053520
N1	H16	5.551598	0.660900	0.032880
N2	H18	5.603725	0.312900	0.097000
N1	C8	5.603866	0.386700	0.011490
N3	H17	5.606041	0.166200	0.083900
N1	H13	5.633069	0.213900	0.008320
N2	H17	5.978465	0.220500	0.087010
N1	H18	6.235056	0.504400	0.124880
N1	H17	6.620525	0.370600	0.071850

Table S8 Least-squares correlation matrix (×100) from the refinement of AMP

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	k_1 [a]	100																
2	k_2 [a]	**52**	100															
3	N1-N2	30	22	100														
4	N2-N3	20	45	-14	100													
5	C4-N3	-10	-4	-15	9	100												
6	C4-N5	-27	-31	-32	34	-32	100											
7	C6-N5, C7-N5 [b]	6	-3	17	-16	**-99**	27	100										
8	C6-C8, C7-C9, C8-C9 [b]	24	37	-2	42	**-62**	**52**	**53**	100									
9	C-H [b]	-39	-28	**-65**	28	20	43	-22	-4	100								
10	C4-N3-N2, N3-C4-N5 [b]	2	-1	16	-20	**-86**	20	**86**	46	-25	100							
11	C4-N5-C6, C4-N5-C7 [b]	10	12	3	7	42	-36	-42	-33	6	**-66**	100						
12	C8-C6-N5	16	23	2	-6	**71**	**-63**	**-71**	**-53**	-8	**-51**	9	100					
13	N1-N2-N3-C4	5	2	6	-4	1	-5	0	-5	-6	0	-26	16	100				
14	N2-N3-C4-N5	8	16	0	13	44	-21	-44	-21	5	**-67**	47	37	23	100			
15	C6-N5-C4-N3, C7-N5-C4-N3 [b]	10	9	-19	20	37	-2	-39	-9	26	**-71**	**75**	-2	-7	49	100		
16	C7-N5-C6-C8	5	8	24	16	**-76**	39	**75**	**62**	-20	**76**	-38	**-71**	-15	**-52**	**-50**	100	
17	C6-C8-C7-C9	1	2	8	30	-33	40	31	40	6	13	17	**-64**	-25	-15	15	**67**	100

[a] k_1 and k_2 are the scale factors. [b] These parameters were refined in the group.

Table S9 Experimental coordinates of atoms (in Å) for three conformers of AMP

№	Atom	X	Y	Z
			gauche-gauche	
1	N	0.28812	0.97930	3.17806
2	N	0.25457	0.13065	2.39112
3	N	0.31410	-0.81966	1.60686
4	C	-0.81563	-0.96790	0.63086
5	N	-0.61477	-0.43337	-0.64980
6	C	-0.38456	1.02099	-0.74552
7	C	0.50249	-0.99909	-1.43559
8	C	-0.11768	1.21162	-2.24924
9	C	0.57864	-0.11161	-2.70029
10	H	-0.89346	-2.04711	0.46597
11	H	-1.73690	-0.59898	1.10421
12	H	-1.26143	1.57758	-0.38913
13	H	0.49434	1.32774	-0.14542
14	H	0.29716	-2.04661	-1.68984
15	H	1.44429	-0.95922	-0.85741
16	H	-1.06664	1.34539	-2.78016
17	H	0.50693	2.08959	-2.44789
18	H	0.05375	-0.58222	-3.53849
19	H	1.61796	0.04786	-3.00800
			gauche-anti	
1	C	0.07872	1.16434	-1.25531
2	C	0.27611	0.78129	-2.73651
3	C	0.27611	-0.78129	-2.73651
4	C	0.07872	-1.16434	-1.25531
5	N	-0.64672	0.00000	-0.70617
6	C	-0.88007	0.00000	0.66832
8	N	0.38773	0.00000	1.47983
9	N	0.24504	0.00000	2.70289
10	N	0.20045	0.00000	3.86010
11	H	-0.52013	2.07715	-1.14179
12	H	1.04039	1.30868	-0.72850
13	H	-0.55215	1.16485	-3.34229
14	H	1.20532	1.19923	-3.13919
15	H	-0.55215	-1.16485	-3.34229
16	H	1.20532	-1.19923	-3.13919
17	H	-0.52013	-2.07715	-1.14179
18	H	1.04039	-1.30868	-0.72850
19	H	-1.45452	0.89939	0.93393
20	H	-1.45452	-0.89939	0.93393
			anti-gauche	
1	N	0.80521	-1.02415	-2.90100
2	N	0.12939	-0.26057	-2.36091
3	N	-0.69463	0.52995	-1.87988
4	C	-0.27652	1.20617	-0.65202
5	N	0.10220	0.31110	0.38328
6	C	0.63737	0.98430	1.58504

7	C	-1.00342	-0.50049	0.93507
8	C	0.71789	-0.16008	2.61603
9	C	-0.38648	-1.17300	2.17876
10	H	-1.14558	1.82607	-0.36472
11	H	0.58045	1.86727	-0.85396
12	H	1.61421	1.43694	1.37411
13	H	-0.05136	1.78618	1.92554
14	H	-1.34822	-1.24131	0.20516
15	H	-1.86373	0.15119	1.19711
16	H	1.70366	-0.63571	2.57373
17	H	0.56682	0.20623	3.63754
18	H	-1.13571	-1.33102	2.96242
19	H	0.03030	-2.15079	1.91450

Fig. S1 Experimental intensity curve with final background for long camera distance

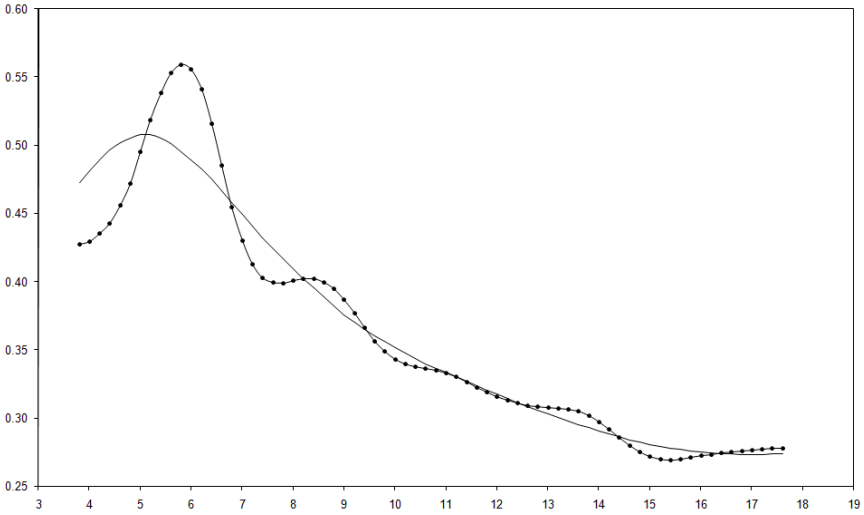


Fig. S2 Experimental intensity curve with final background for short camera distance