

Neighbouring Effect on Fragmentation Pathways of Cage Guanylhyazones in the Gas Phase

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SUPPORTING INFORMATION

¹³C NMR spectrum of compound 10b in CDCl₃. The spectrum displays several peaks corresponding to different carbon environments. Key peaks are labeled as follows:

- isomer A: 110.2 ppm
- isomer B: 100.3 ppm
- isomer C: 90.0 ppm
- Aromatic/Aliphatic region (40-60 ppm): Multiple peaks labeled with values including 162.2, 160.1, 158.9, 158.7, 158.3, 156.1, 155.7, 49.3, 43.2, 42.5, 42.1, 39.7, 39.1, 37.6, 37.0, 36.9, 35.9, 35.3, 34.0, 31.1, 26.4, and 26.3 ppm.

Table S1. Electronic, zero-point and total energies and relative stabilities of all stationary points calculated at B3LYP/6-311+G(d,p) and BMK/6-311+G(3df,2p) (values in parentheses) levels of theory.

Molecule	$E_{\text{SCF}} / \text{a.u.}$	$E_{\text{ZPV}} / \text{a.u.}$	$E_{\text{tot}} / \text{a.u.}$	$E_{\text{rel}}^{\text{a}} / \text{kcal mol}^{-1}$
NH₃	-56.58264 (-56.54394)	0.03423	-56.54841 (-56.50972)	-
CH₂N₂	-148.83410 (-148.75052)	0.03259	-148.80151 (-148.71793)	-
CH₅N₃	-205.44624 (-205.33109)	0.07580	-205.37044 (-205.25529)	-
1H⁺	-649.59155 (-649.21183)	0.30330	-649.28825 (-648.90853)	0.0 (0.0)
TS_A1	-649.51196 (-649.12752)	0.29961	-649.21235 (-648.82791)	47.6 (50.6)
1a_im	-649.53954 (-649.15581)	0.30507	-649.23447 (-648.85074)	33.8 (36.3)
TS_A2	-649.52144 (-649.12807)	0.29910	-649.22234 (-648.82898)	41.4 (49.9)
1ah_NH₃	-649.53781 (-649.14389)	0.29836	-649.23945 (-648.84553)	30.6 (39.5)
1aH⁺	-592.92211 (-592.57063)	0.26147	-592.66064 (-592.30916)	- -
1aH⁺ + NH₃	-649.50474 (-649.11457)	0.29570	-649.20904 (-648.81888)	49.7 (56.3)
TS_B1	-649.56341 (-649.18047)	0.30047	-649.26295 (-648.88000)	15.9 (17.9)
1b_im	-649.57037 (-649.18880)	0.30501	-649.26537 (-648.88379)	14.4 (15.5)
TS_B2	-649.49091 (-649.09555)	0.29928	-649.19164 (-648.79628)	60.6 (70.4)
1bH_NH₃	-649.55220 (-649.16119)	0.30053	-649.25165 (-648.86067)	23.0 (30.0)
1bH⁺	-500.69751 (-500.39175)	0.26643	-500.43108 (-500.12533)	- -
1bH⁺ + CH₂N₂	-649.53161 (-649.14227)	0.29902	-649.23259 (-648.84325)	34.9 (41.0)
TS_C1	-649.51092 (-649.21183)	0.29732	-649.21360 (-648.90853)	46.9 (55.3)
1c_{tc}⁺ (min 1)	-444.05410 (-443.77592)	0.22055	-443.83355 (-443.55537)	^b ^b
(min 2)	-444.05690 (-443.78469)	0.22357	-443.83334 (-443.56113)	53.0 ^c (57.8) ^c
TS_C3	-444.02977 (-443.74971)	0.21524	-443.81454 (-443.53447)	64.8 ^c (74.5) ^c
1cH⁺	-444.06652 (-443.78820)	0.22019	-443.84633 (-443.56801)	- -
1cH⁺ + CH₅N₃	-649.51276 (-649.11929)	0.29598	-649.21678 (-648.82330)	44.9 (53.5)

a) Relative stabilities (E_{rel}) of all stationary points except for the Pathway C were calculated with respect to the starting monocation **1H⁺**; b) two minima of the similar structures were located with the barrier for their interconversion of only 0.7 kcal mol⁻¹. Two DFT (B3LYP and BMK) approaches predict different trend in their stabilities; c) $E_{\text{rel}}(\text{X}) = E_{\text{tot}}(\text{X}) + E_{\text{tot}}(\text{CH}_5\text{N}_3) - E_{\text{tot}}(\text{1H}^+)$; **X** = **1c_{tc}⁺** or **TS_C3**.

Table S2. Electronic, zero-point and total energies and relative stabilities of all stationary points calculated at B3LYP/6-311+G(d,p) levels of theory.

Molecule	$E_{\text{SCF}} / \text{a.u.}$	$E_{\text{ZPV}} / \text{a.u.}$	$E_{\text{tot}} / \text{a.u.}$	$E_{\text{rel}}^{\text{a}} / \text{kcal mol}^{-1}$
3H⁺	-907.96536	0.35217	-907.61319	0.0
3aH⁺	-851.33011	0.31011	-851.02000	28.1
3bH⁺	-759.08021	0.31310	-758.76711	28.0
3cH⁺	-702.43357	0.26829	-702.16529	48.6
4H⁺	-907.97932	0.35387	-907.62545	0.0
4aH⁺	-851.33602	0.31220	-851.02382	33.4
4bH⁺	-759.08713	0.31465	-758.77248	32.3
4cH⁺	-702.48020	0.27068	-702.20952	28.5
5H⁺	-944.81672	0.33460	-944.48211	0.0
5aH⁺	-888.18125	0.29244	-887.88881	28.2
5bH⁺	-795.93208	0.29558	-795.63651	27.7
5cH⁺	-739.33261	0.25417	-739.07845	20.9

a) Relative stabilities (E_{rel}) were calculated with respect to the starting monocations **3H⁺**, **4H⁺** or **5H⁺**.

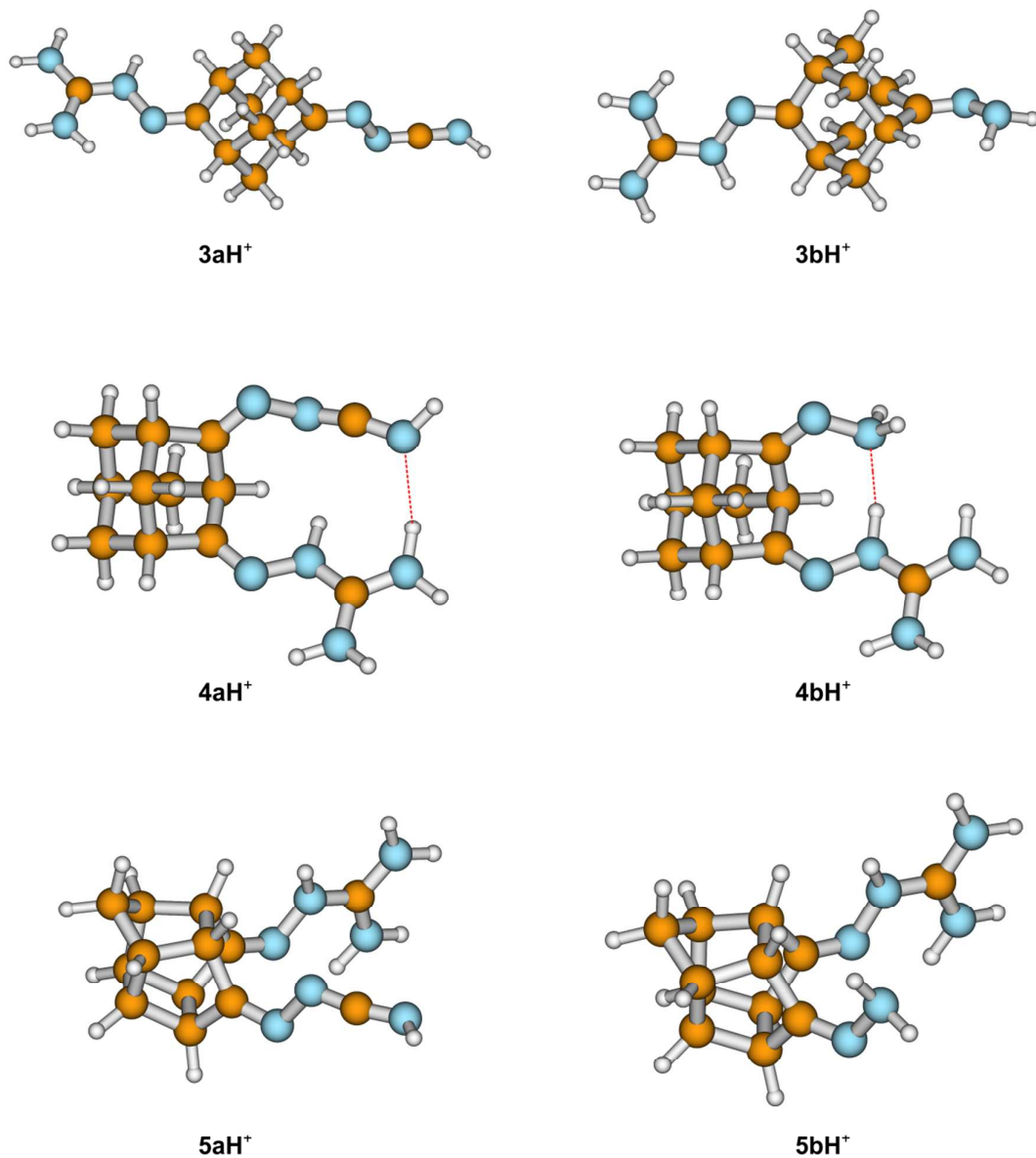


Figure S3. Calculated structures of the products obtained by fragmentation of parent ions **3H⁺**-**5H⁺** via Pathways A and B optimized at the B3LYP/6-311+G(d,p) level of theory.

Table S3. Calculated geometries at the stationary points.

1

C	0.2994267787	-0.4043943790	0.5039664500
C	0.0230580028	0.0444947219	1.9209643402
N	1.5128617194	-0.5734433649	0.1264240505
C	-0.7183470440	1.4039187031	1.8667469151
C	-0.8861920454	-1.0031072080	2.6096573156
H	0.9715283322	0.1430487674	2.4544085053
C	-2.0260805929	1.2484085187	1.0648760496
H	-0.9349447980	1.7449072828	2.8860472755
H	-0.0746457882	2.1593048796	1.4032272367
C	-1.6952973264	0.7819596492	-0.3671612871
C	-2.9256115159	0.1997995699	1.7514757684
H	-2.5476272023	2.2111080604	1.0250415592
C	-0.9577198197	-0.5800313039	-0.3225263855
H	-2.6159025391	0.6773409967	-0.9535401413
H	-1.0734006997	1.5264452627	-0.8754899172
C	-1.8624014011	-1.6246040585	0.3784782917
H	-0.6919735212	-0.9082768771	-1.3259962981
H	-3.8678639848	0.0950056251	1.2007887824
C	-2.1945946528	-1.1574566913	1.8094442595
H	-3.1836855609	0.5305437934	2.7645066193
H	-1.3595569565	-2.5972675346	0.4020811639
H	-2.7836669729	-1.7530307865	-0.2021658045
H	-1.1027745941	-0.6836885049	3.6358752434
H	-0.3642556839	-1.9640513748	2.6740610682
H	-2.8362825928	-1.9000900879	2.2963642222
N	1.6961710535	-0.9830206602	-1.1964527651
C	2.9516485953	-1.0163318154	-1.5190404407
N	3.3163908635	-1.5546257774	-2.7438041440
N	3.9906052885	-0.5486317474	-0.7457023244
H	2.5142089167	-1.760259978	-3.3237983444
H	4.0399457667	-1.0464360238	-3.2348545137
H	3.6869071396	-0.3391920412	0.1986820560
H	4.8565058356	-1.0635696164	-0.8133598067

1H⁺

C	0.2629821624	-0.3397224444	0.4837159465
C	0.0084234628	0.0956475595	1.9053567336
N	1.4852861712	-0.4936521164	0.1183635284
C	-0.7706075575	1.4365634267	1.8729196017
C	-0.8585712647	-0.9871909806	2.5994202349
H	0.9642287657	0.2150131630	2.4192783669
C	-2.0910211126	1.2489382007	1.1035813061
H	-0.9649982786	1.7549543534	2.9014520051
H	-0.1598722690	2.2167683170	1.4067444341
C	-1.7736773037	0.8131133892	-0.3395034330
C	-2.9488723391	0.1697377424	1.7944691606
H	-2.6365316945	2.1964742402	1.0785628741
C	-1.0009488517	-0.5349539648	-0.3207276620

H	-2.6949368812	0.6774034337	-0.9142972316
H	-1.1847072557	1.5813625587	-0.8514491186
C	-1.8618736732	-1.6166696576	0.3887902359
H	-0.8080326870	-0.8510151217	-1.3516587359
H	-3.8977304178	0.0447359096	1.2625525524
C	-2.1786561130	-1.1657720387	1.8273581514
H	-3.1959354965	0.4840827611	2.8132885387
H	-1.3356519150	-2.5769993075	0.3949514422
H	-2.7833442453	-1.7581293727	-0.1842774320
H	-1.0531635370	-0.6743672889	3.6296227233
H	-0.3105171757	-1.9337793785	2.6508491850
H	-2.7863760075	-1.9324421696	2.3161558366
N	1.7400451348	-0.8956270260	-1.1917804152
C	3.0173282912	-1.0517329774	-1.5573609005
N	3.3126975358	-1.4369362482	-2.8088005580
N	3.9726869295	-0.8189545266	-0.6625795971
H	2.5930762733	-1.6164253853	-3.4904516435
H	4.2673810214	-1.5617663533	-3.1049821357
H	3.6795300223	-0.5305253405	0.2626945328
H	4.9505779088	-0.9192562465	-0.8800254984
H	0.991653397	-1.0657111097	-1.8537090287

TS_A1

C	0.2624205943	-0.3214904569	0.5644790201
C	-0.0392846363	0.1066515274	1.9747528117
N	1.5006231461	-0.4780349160	0.2337835312
C	-0.8184135758	1.4484763085	1.9190582136
C	-0.9346110608	-0.9788654708	2.6310178945
H	0.8965634581	0.2231522870	2.5246338345
C	-2.1080876312	1.2641531948	1.0988134713
H	-1.0504541299	1.7614757621	2.9415435148
H	-0.1904116921	2.2305840840	1.4797476030
C	-1.7355956091	0.8332375692	-0.3318067759
C	-2.9917255804	0.1830689915	1.7533553613
H	-2.6519458812	2.2123974138	1.0585494850
C	-0.9612465219	-0.5140768031	-0.2920472243
H	-2.6339949653	0.6990139242	-0.9423406532
H	-1.1288875142	1.6041300103	-0.8185994665
C	-1.8519016630	-1.5960159173	0.3807141968
H	-0.6911690689	-0.8232927976	-1.3022225520
H	-3.9199629562	0.0609278051	1.1854525929
C	-2.2238160171	-1.1530914351	1.8078216269
H	-3.2769240613	0.4930873271	2.7637668483
H	-1.3281464508	-2.5575567638	0.4020569163
H	-2.7504615357	-1.7335995862	-0.2288338547
H	-1.1667930934	-0.6695935838	3.6546055005
H	-0.3894091932	-1.9260857969	2.6988394456
H	-2.8498558731	-1.9212692737	2.2710153067
N	1.7611685128	-0.8724680033	-1.0677517484
C	3.0056225849	-1.0301161817	-1.4011738091
N	2.8864765586	-1.4327890619	-2.7916649473

N	4.1308357467	-0.8827611954	-0.7124097017
H	3.1884083410	-2.3852830705	-3.0041126469
H	3.2655947404	-0.7767001689	-3.4767557947
H	4.0425991271	-0.5937649526	0.2551169258
H	5.0454836093	-1.0392433312	-1.1035285664
H	1.6571742915	-1.2610924383	-2.4073513596

1a_im

C	0.3516527536	-0.6145792503	1.0037627284
C	-0.1037974651	0.2280104545	2.1640942226
N	1.6118215220	-0.8896504999	0.9169193980
C	-0.7704523290	1.5111661263	1.5983761851
C	-1.1532523632	-0.5803343011	2.9735784862
H	0.7568017251	0.4801060776	2.7867780123
C	-1.9504610076	1.1234156005	0.6886982394
H	-1.1118609607	2.1272572279	2.4359216016
H	-0.0351166276	2.1036703062	1.0439288817
C	-1.4235468340	0.2667523460	-0.4773876104
C	-2.9873532777	0.3175291686	1.4972405874
H	-2.4154852528	2.0298732868	0.2899559756
C	-0.7588756104	-1.0255541495	0.0732600258
H	-2.2409248459	-0.0207075713	-1.1463225690
H	-0.7042492993	0.8357720456	-1.0759253318
C	-1.8054688176	-1.8253681711	0.8980074965
H	-0.3713621678	-1.6323753156	-0.7438349868
H	-3.8386992863	0.0546540209	0.8605629034
C	-2.3312715268	-0.9602647492	2.0582311382
H	-3.3808634420	0.9274830036	2.3168789396
H	-1.3590522420	-2.7495306836	1.2801930411
H	-2.6233068693	-2.1166064266	0.2311812546
H	-1.4963101043	0.0319659502	3.8132522130
H	-0.6909902666	-1.4771125849	3.3993539858
H	-3.0668698361	-1.5329034674	2.6308436382
N	1.9729656735	-1.6749716933	-0.1860562480
C	3.2278907395	-1.8563537988	-0.2361169324
N	3.6424047110	-2.6855558675	-1.4095725448
N	4.2480469657	-1.3264683478	0.4873342333
H	2.7692828535	-2.9278677650	-1.8959813153
H	4.2526037749	-2.1606326076	-2.0485431049
H	3.9022186698	-0.7834129235	1.2749457044
H	4.1229328792	-3.5529550226	-1.1434634905
H	5.0843601642	-1.8639054178	0.6722462417

TS_A2

C	-0.0148801888	0.2799751830	-0.0177346997
C	0.9866045095	1.3911061695	0.1151551283
N	-1.2666632603	0.6035491805	0.0079143851
C	1.8150318847	1.1236264042	1.4036456885
C	1.9275806224	1.3493849016	-1.1199048086
H	0.4667885577	2.3488101114	0.1790409656
C	2.4966102324	-0.2533244674	1.3043376709

H	2.5584555109	1.9193439692	1.5077464229
H	1.1670261174	1.1733259431	2.2846852497
C	1.4169170294	-1.3431819466	1.1647962758
C	3.4284843533	-0.2857024595	0.0762625061
H	3.0757120310	-0.4366835437	2.2139378550
C	0.5838199431	-1.0919460385	-0.1247005245
H	1.8720315281	-2.3354755692	1.0931146397
H	0.7635983698	-1.3520399904	2.0435212522
C	1.5292258049	-1.1127309742	-1.3588905046
H	-0.2014502921	-1.8442689990	-0.2280774385
H	3.9321802003	-1.2556618144	0.0117185911
C	2.6106472738	-0.0274848767	-1.2047180804
H	4.2125657422	0.4711313337	0.1793629402
H	0.9546641830	-0.9575208091	-2.2777434055
H	1.9810850234	-2.1068030589	-1.4278416941
H	2.6695750859	2.1464885145	-1.0162857956
H	1.3612555623	1.5567095382	-2.0336642872
H	3.2699997883	-0.0518032558	-2.0769284124
N	-2.1604092791	-0.4319903800	-0.1298417391
C	-3.3250516874	-0.6016444210	0.0044426259
N	-4.2574319349	1.5322638338	-0.2803872947
N	-4.4024144403	-1.3075490622	0.1927472683
H	-3.3814929240	2.0420395698	-0.1818798523
H	-4.6369143491	1.7559398965	-1.1972879646
H	-4.3747178954	-2.1440718281	0.7627949315
H	-4.9026777459	1.8916210516	0.4189080763
H	-5.2905543564	-0.9766431056	-0.1555289714

1aH⁺

C	0.3520466657	-0.3056009283	1.4342393562
C	-0.4108730515	0.4597283394	2.4681497333
N	1.6382025319	-0.4047767828	1.6237063982
C	-1.1285347587	1.6427033505	1.7545859453
C	-1.4779532083	-0.4970327298	3.0766351941
H	0.2739302925	0.8222747180	3.2361684227
C	-2.0471824512	1.0975437230	0.6473992361
H	-1.7020263487	2.1953327796	2.5040207434
H	-0.3898249256	2.3367905337	1.3416905799
C	-1.1932693395	0.3346408927	-0.3802119468
C	-3.0999008461	0.1508115340	1.2577949834
H	-2.5452704699	1.9329097390	0.1471820288
C	-0.4734253673	-0.8597210667	0.3166006743
H	-1.8138272202	-0.0679730763	-1.1860481632
H	-0.4586939108	1.0013433258	-0.8431113534
C	-1.5431516448	-1.8058343828	0.9418361309
H	0.1496209168	-1.4027100271	-0.3975244395
H	-3.7684934872	-0.2231264016	0.4757395932
C	-2.3939609168	-1.0266082746	1.9596677147
H	-3.7241941853	0.6949086090	1.9733132778
H	-1.0577676201	-2.6627256237	1.4198635789
H	-2.1625507669	-2.1992676502	0.1306014568

H	-2.0505144313	0.0613310059	3.8225525063
H	-0.9870849867	-1.3220394196	3.6023413964
H	-3.1386316246	-1.7007102826	2.3923791655
N	2.3087893400	-1.1102635246	0.6656909430
C	3.3262800830	-1.5268677824	0.2791563732
N	4.3843802517	-2.0433252607	-0.2595003119
H	4.9668735627	-1.4965527348	-0.8837427051
H	4.7031989169	-2.9676296018	0.0087224874

1aH_nh3 (1aH⁺ + NH₃; H-bond associate)

C	0.344974	0.513447	0.222072
C	1.548032	1.406808	0.310711
N	-0.809777	1.077655	0.385713
C	2.430852	0.896793	1.484615
C	2.339170	1.283516	-1.020494
H	1.226734	2.435381	0.482564
C	2.824835	-0.570703	1.237547
H	3.318481	1.532697	1.550060
H	1.892711	1.000031	2.432271
C	1.547708	-1.427501	1.158696
C	3.609953	-0.683555	-0.084535
H	3.443010	-0.924660	2.067557
C	0.656201	-0.934133	-0.018136
H	1.793210	-2.479503	0.985053
H	0.992530	-1.378028	2.101089
C	1.458458	-1.039316	-1.346671
H	-0.262775	-1.520975	-0.076099
H	3.911541	-1.722013	-0.256187
C	2.735662	-0.185476	-1.253020
H	4.529928	-0.093149	-0.026013
H	0.838833	-0.715309	-2.189060
H	1.704142	-2.092036	-1.515641
H	3.225335	1.921786	-0.956431
H	1.735732	1.658184	-1.853655
H	3.291041	-0.266772	-2.191817
N	-1.890783	0.219495	0.289368
C	-3.038519	0.161140	0.538783
N	-6.133106	1.028018	-1.012570
N	-4.298325	-0.001908	0.686799
H	-5.731725	1.663512	-1.699655
H	-6.619671	0.300760	-1.533430
H	-4.632250	-0.483915	1.515027
H	-6.842807	1.555570	-0.507381
H	-5.035356	0.422469	-0.020764

1bH⁺

C	0.2465539232	-0.5697794614	0.8288066057
C	-0.0631760373	0.2757886932	2.0171990942
N	1.4842534365	-0.8678672133	0.5487106807
C	-0.8224249153	1.5402157848	1.5098991765
C	-1.0002131443	-0.5502693459	2.9510804352

H	0.8529509492	0.5611766223	2.5441775678
C	-2.0871064356	1.1080915055	0.7482293261
H	-1.0722708137	2.1505298008	2.3818001196
H	-0.1693138411	2.1443466363	0.8723046420
C	-1.6722600520	0.2528616824	-0.4608451628
C	-3.0071889545	0.2930150159	1.6789722216
H	-2.6121207016	1.9993402734	0.3940336422
C	-0.9171679646	-1.0246333158	0.0254976842
H	-2.5449156466	-0.0790507719	-1.0294440504
H	-1.0426823034	0.8256285443	-1.1487260224
C	-1.8499461180	-1.8362663981	0.9794064803
H	-0.5878049319	-1.6320733073	-0.8149686243
H	-3.9180531051	0.0034808427	1.1466353151
C	-2.2632184272	-0.9627009787	2.1758340044
H	-3.3194513117	0.9060813178	2.5297603635
H	-1.3466297986	-2.7482051486	1.3150387372
H	-2.7209641799	-2.1490919266	0.3976261107
H	-1.2486819491	0.0762535269	3.8118073249
H	-0.4732350838	-1.4290881375	3.3358272680
H	-2.9133913981	-1.5429827360	2.8361105665
N	1.8483857231	-1.6609361307	-0.5569517624
H	2.4590461972	-1.1235400117	-1.1672441546
H	2.2179654131	-0.5089125230	1.1600035365
H	2.3437504710	-2.4858978400	-0.2280171259

TS_B1

C	0.2715588945	-0.6174010321	0.8444013469
C	-0.0486463965	0.2417930442	2.0344962644
N	1.4951144849	-0.9276915060	0.6076988066
C	-0.7679616990	1.5200733242	1.5215927300
C	-1.0115608150	-0.5620716510	2.9520317695
H	0.8688121248	0.5017362363	2.5676247019
C	-2.0353457158	1.1235028734	0.7418412803
H	-1.0204433516	2.1431478683	2.3841358400
H	-0.0924035088	2.1069678358	0.8907360013
C	-1.6313570552	0.2591202480	-0.4677614303
C	-2.9845683332	0.3260428400	1.6582357075
H	-2.5363716768	2.0269466251	0.3836932418
C	-0.9163226661	-1.0315590414	0.0257878932
H	-2.5106673290	-0.0365847370	-1.0471419379
H	-0.9788276625	0.8239150031	-1.1421424487
C	-1.8723427123	-1.8260948077	0.9637720299
H	-0.6219997215	-1.6584944050	-0.8185005478
H	-3.8962286777	0.0588331264	1.1144443039
C	-2.2752800667	-0.9471668756	2.1614776238
H	-3.2933283976	0.9440471981	2.5070638824
H	-1.3881662471	-2.7470677886	1.3032172932
H	-2.7504150315	-2.1211129825	0.3820538196
H	-1.2661023378	0.0610265187	3.8141329931
H	-0.5086796583	-1.4541636719	3.3387536344
H	-2.9482173879	-1.5143316929	2.8104772613

N	1.9188267514	-1.7495091327	-0.4493596900
C	3.3228190363	-1.8723782185	-0.3349761439
N	3.9514476114	-2.5218147393	-1.3292883007
N	3.7915939307	-1.3209387090	0.7326926802
H	3.4292147255	-3.1093265945	-1.9621990004
H	4.9449926423	-2.6842579193	-1.2736461368
H	4.7661662784	-1.4106355427	0.9834275196
H	1.5775073967	-1.4793831518	-1.3661693976
H	2.6141455708	-0.8080165421	1.1321234095

1b_im

C	0.2763113042	-0.5555939413	0.8470173993
C	-0.0602955220	0.2857158272	2.0380770155
N	1.5113529617	-0.8325270579	0.5875500069
C	-0.8179300900	1.5458435765	1.5273853618
C	-1.0023887523	-0.5522387797	2.9512699143
H	0.8476078163	0.5717012575	2.5761311046
C	-2.0697658542	1.1115999200	0.7436335272
H	-1.0893833849	2.1533303521	2.3948281932
H	-0.1588696234	2.1570110710	0.9025544811
C	-1.6368196164	0.2661262031	-0.4685906784
C	-2.9970666134	0.2828516105	1.6548811505
H	-2.5966785142	2.0008967987	0.3875202934
C	-0.8826248141	-1.0067513144	0.0218831491
H	-2.5035008198	-0.0588822516	-1.0505897039
H	-1.0012736012	0.8517855956	-1.1409797291
C	-1.8182637868	-1.8331109642	0.9570410753
H	-0.5573896728	-1.6190603796	-0.8201960949
H	-3.8985984606	-0.0092682717	1.1075031660
C	-2.2516561408	-0.9705906561	2.1551714335
H	-3.3266871280	0.8883110436	2.5046954774
H	-1.3081670276	-2.7408737286	1.2932234046
H	-2.6826063631	-2.1508480034	0.3674296248
H	-1.2737772531	0.0633153694	3.8132594912
H	-0.4733087102	-1.4291095911	3.3370451539
H	-2.9081915740	-1.5599966893	2.8008953568
N	1.9755856964	-1.6331061107	-0.4585661014
C	3.3796667046	-1.8922423373	-0.2976057266
N	3.8860520271	-2.5887365413	-1.3540658239
N	3.9336545955	-1.4254435159	0.7476427918
H	3.2783386583	-3.2151626983	-1.8624947036
H	4.8558314084	-2.8641185462	-1.3170054087
H	4.9039535761	-1.6859159514	0.8851506694
H	1.7492019110	-1.2355925624	-1.3663500409
H	2.3146546634	-0.5821647326	1.1993847699

TS_B2

C	0.0446378104	-0.0329154636	-0.6392658382
C	-1.0927770634	0.6942858090	-1.2972717948
N	1.2139754406	-0.0874011263	-1.2133440834
C	-2.2490622294	-0.3175771659	-1.5241621396

C	-1.5704062070	1.8129806688	-0.3315069784
H	-0.7715231557	1.1257119836	-2.2522438928
C	-2.6585255281	-0.9353689041	-0.1731638453
H	-3.0934924059	0.2069141244	-1.9809013506
H	-1.9365792186	-1.0975277516	-2.2259650394
C	-1.4506194401	-1.6716752741	0.4372319773
C	-3.1278980498	0.1773224423	0.7856576951
H	-3.4691961898	-1.6513063237	-0.3348077231
C	-0.2881300578	-0.6646865521	0.6774642588
H	-1.7191740686	-2.1265561467	1.3952944969
H	-1.1183256358	-2.4805833069	-0.2210437418
C	-0.7722745979	0.4622809938	1.6339266397
H	0.5696605138	-1.1825622873	1.1123216940
H	-3.4423948614	-0.2566581656	1.7402851353
C	-1.9833043383	1.1853565059	1.0141019023
H	-4.0013628785	0.6885282089	0.3684583814
H	0.0406470057	1.1700982705	1.8270264586
H	-1.0414020667	0.0127993735	2.5943131315
H	-2.4150844525	2.3372936167	-0.7880384154
H	-0.7747427277	2.5510311614	-0.1854632161
H	-2.3160411350	1.9752328859	1.6934190851
N	2.3933864408	-0.6700855122	-0.8605908416
C	4.6125121135	0.4287589302	-0.9976763801
N	4.7734545306	-0.6316383766	-1.6975171769
N	4.7563453522	1.5232088117	-0.5660635108
H	3.8851409186	-1.1718519667	-1.7886032602
H	5.6957419128	-0.9282951098	-1.9999800887
H	4.7404165853	1.9422850476	0.3516210011
H	2.2463201724	-1.1326256249	0.0354778196
H	1.2790455110	0.3794892242	-2.1148413595

1bH_cdi (1bH⁺ + CH₂N₂; H-bond associate)

C	0.2626864181	-0.4806869295	-0.0487333862
C	-0.3491486234	0.5333422452	-0.9611349204
N	1.5072412668	-0.8182021323	-0.1994607061
C	-1.5597451639	-0.1418040974	-1.6725959749
C	-0.8621462522	1.7110951036	-0.0794203055
H	0.3815182274	0.8872954275	-1.6926181486
C	-2.5547163718	-0.6603278290	-0.6198431149
H	-2.0257950535	0.6033775920	-2.3231166008
H	-1.2144688817	-0.9572056733	-2.3163041871
C	-1.8473188407	-1.7010955077	0.2645260104
C	-3.0558126099	0.5119200999	0.2475338483
H	-3.3994828009	-1.1338224150	-1.1277069697
C	-0.6383199694	-1.0416865525	0.9962255641
H	-2.5233032035	-2.0951587868	1.0282834654
H	-1.5088775444	-2.5543038329	-0.3317720047
C	-1.1515055687	0.1525807693	1.8587600062
H	-0.1052010638	-1.7669879851	1.6073726958
H	-3.7797540018	0.1509624582	0.9845382568
C	-1.8628273189	1.1790288840	0.9610537873
H	-3.5782308586	1.2441643672	-0.3759293199
H	-0.3185247096	0.6148717324	2.3976632688
H	-1.8328620614	-0.2514369476	2.6123853322
H	-1.3314767464	2.4456258943	-0.7396384999
H	-0.0210270013	2.2126178571	0.4098195325
H	-2.2167094627	2.0110805117	1.5760035364
N	2.1292435797	-1.7743915288	0.6377220995
C	3.8841216471	1.3688416412	-2.1333617203
N	3.3307089669	0.2639192858	-2.2112347487
N	4.2430767320	2.5106084730	-2.0022594746
H	2.9422963862	-1.3403153973	1.0682147936
H	3.4718846759	-0.2512861255	-3.0765854287
H	5.1429379381	2.8118841247	-1.6513471350
H	2.4527403668	-2.5453943752	0.0579739175
H	2.0840009034	-0.3834303514	-0.9483204689

1cH⁺

C	0.4829415050	-1.0380733157	0.4406019629
C	-0.4519527444	0.7608239083	2.6627720296
N	1.6218846436	-1.0375574776	0.5950232987
C	-0.9732971423	1.7077894734	1.6114611730
C	-1.0106121515	-0.4263848083	2.9328988080
H	0.3966584794	1.0986327424	3.2525390276
C	-2.0578438047	1.0773185851	0.7150569402
H	-1.3855488909	2.5896053664	2.1177897099
H	-0.1454627526	2.0974265423	1.0056145438
C	-1.4970452011	0.2164455333	-0.4349741734
C	-3.0088201528	0.2334255601	1.5804649010
H	-2.6170960716	1.8857265481	0.2358377099
C	-0.8923465945	-1.1592082402	0.0076430370

H	-2.3146102509	-0.0459594737	-1.1123067890
H	-0.7674829993	0.7726804767	-1.0295939910
C	-1.7747888808	-1.9009757020	1.0552538748
H	-0.7936756183	-1.7971592604	-0.8833655029
H	-3.8501343753	-0.1367083009	0.9861739857
C	-2.2175145515	-0.9409526116	2.1810960115
H	-3.4283763485	0.8460336464	2.3820383028
H	-1.2452548558	-2.7713585995	1.4505244197
H	-2.6467697363	-2.2758842374	0.5120974036
H	-0.5991186315	-1.0516182392	3.7209395242
H	-2.8529602991	-1.5120975648	2.8636394656
H	2.5901654257	-0.9820405512	0.8642053267

TS_c1

C	0.3471474486	-0.3754066381	0.8350388962
C	-0.3248459616	0.9264746378	2.2277096109
N	1.4284409628	-0.0027743276	1.1009094648
C	-1.1682716534	1.7671781593	1.3161504033
C	-1.0158224102	-0.0710550462	3.1091598928
H	0.5527047431	1.4071598563	2.6463010647
C	-2.3053055912	0.9755436216	0.6362288698
H	-1.5959702222	2.5320877294	1.9859973477
H	-0.5475502464	2.3157571409	0.6032564136
C	-1.7304059928	0.0107724463	-0.4192924828
C	-3.0919056197	0.1838550629	1.7006482446
H	-2.9659484440	1.6882669549	0.1378409435
C	-0.8234542499	-1.0509496747	0.2476208139
H	-2.5435791140	-0.5172216046	-0.9239174391
H	-1.1754613237	0.5537452206	-1.1889657886
C	-1.5825162363	-1.8116334427	1.3606814490
H	-0.3893958645	-1.7335606969	-0.4902111979
H	-3.9261228783	-0.3441867296	1.2305967014
C	-2.1570980224	-0.8266013000	2.3965026860
H	-3.5293179951	0.8663497997	2.4363630430
H	-0.9258161331	-2.5448415611	1.8367190522
H	-2.3940519567	-2.3696690824	0.8868137745
H	-1.4301880765	0.5438928643	3.9258338273
H	-0.2945648800	-0.7409798827	3.5842334247
H	-2.7129901750	-1.3915183898	3.1480113531
N	2.3216027895	-1.5436325900	-0.8982008710
C	3.4379681853	-2.1822704532	-0.7329913497
N	4.6475542231	-1.8548800773	-1.3032066149
N	3.4823617189	-3.2958657850	0.0692762174
H	4.6545817470	-1.1149239360	-1.9871680001
H	5.3081652034	-2.5972314827	-1.4815714898
H	2.6362582782	-3.5023490791	0.5746330725
H	4.3411001143	-3.5065412508	0.5542917807
H	2.4212336329	-0.8128724633	-1.5986991132

1c_{tc}⁺ (min 1)

C	0.30514762	-0.7851697014	0.5105478717
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C	-0.0602498036	0.6181837792	2.3855538007
N	0.8307879681	-0.1966279319	1.3579397455
C	-0.8166278412	1.6366952163	1.5309336221
C	-0.9533001764	-0.4301130842	3.0514122543
H	0.6536125041	1.0720641542	3.0666949025
C	-1.9724821391	1.0396553251	0.6745571905
H	-1.2593463529	2.3459492105	2.2397423463
H	-0.1132006410	2.2145157372	0.9257806867
C	-1.5651166540	0.1730237276	-0.5500473411
C	-2.8996153836	0.2187400503	1.5874492627
H	-2.5212943099	1.8923348689	0.2672928688
C	-0.9136426132	-1.1997206052	-0.1624813365
H	-2.4719401143	-0.0758682266	-1.1090529885
H	-0.9088674660	0.7164623230	-1.2338922552
C	-1.7030433724	-1.9167180831	0.9872195698
H	-0.7519955027	-1.8450637065	-1.0252751774
H	-3.7706267941	-0.1349152405	1.0284371604
C	-2.1053398530	-0.9709915242	2.1535935124
H	-3.2805704986	0.8423764473	2.4010236046
H	-1.1396939726	-2.7833971461	1.3409711111
H	-2.6185182082	-2.2984976767	0.5257960733
H	-1.4097294406	0.0741450472	3.9109743016
H	-0.3414388544	-1.2361886842	3.4646496895
H	-2.7496081000	-1.5625672764	2.8086335242

1c_{tc}⁺ (min 2)

C	0.4139915601	-0.7624344291	0.5514527204
C	-0.2477212883	0.6661453267	2.4339717673
N	1.3456283300	-0.3925081662	1.1380572556
C	-0.8809115827	1.6221985845	1.5108982849
C	-1.0173737840	-0.4394267444	3.0275829710
H	0.6775840905	0.9625304476	2.9201017338
C	-2.0544810725	1.0541306285	0.6764246150
H	-1.2713579243	2.3843970320	2.2172687494
H	-0.1289939414	2.1606972146	0.9275423783
C	-1.5764687464	0.1888568927	-0.5088137693
C	-2.9763470427	0.2282776725	1.5932863950
H	-2.6027252599	1.9047090587	0.2662207981
C	-0.8718103514	-1.1187793294	-0.0485351786
H	-2.4494176809	-0.1036401709	-1.0980785012
H	-0.9209820195	0.7553136310	-1.1749074803
C	-1.7134030475	-1.8810964905	1.0139710665
H	-0.6747900135	-1.7643814665	-0.9084000169
H	-3.8393425768	-0.1309263055	1.0273787605
C	-2.1881831386	-0.9662947733	2.1627603928
H	-3.3722082653	0.8499871188	2.4027872121
H	-1.1520572702	-2.7378395455	1.3948901366
H	-2.5934635860	-2.2813460992	0.5039501033
H	-1.4264028384	0.0423655382	3.9402311185
H	-0.3525993573	-1.2174720249	3.4127904469
H	-2.8320061931	-1.5599456004	2.8149820402

TS_c2

C	0.3659041335	-0.7626316462	0.5471212292
C	-0.1756328708	0.6436618746	2.4100653013
N	1.1704296254	-0.2998700912	1.2478395114
C	-0.8461094456	1.6193668779	1.5058763142
C	-0.9830797374	-0.4463750705	3.0256520634
H	0.6697034232	1.0097629024	2.9838480258
C	-2.0214749088	1.0472394735	0.6720107638
H	-1.2469052942	2.3667654885	2.2138242359
H	-0.1108197283	2.1665686878	0.9105775667
C	-1.5772178790	0.1802101190	-0.5278374309
C	-2.9426512589	0.2262366218	1.5935083798
H	-2.5695135962	1.9009190321	0.2672545739
C	-0.8863685119	-1.1457771377	-0.0865782127
H	-2.4638614015	-0.1003325583	-1.1022687960
H	-0.9235343228	0.7368805629	-1.2037271361
C	-1.7145236225	-1.8966577405	1.0000197998
H	-0.6871591732	-1.7908293790	-0.9455160611
H	-3.8146748160	-0.1258585974	1.0363804677
C	-2.1551561022	-0.9713142277	2.1569026113
H	-3.3249029091	0.8503123599	2.4074373367
H	-1.1543952792	-2.7593941077	1.3687392241
H	-2.6081346596	-2.2855261619	0.5050216327
H	-1.4012271472	0.0425855840	3.9237321133
H	-0.3365739714	-1.2368821083	3.4149932323
H	-2.7988175466	-1.5607557579	2.8135752536

TS_c3

C	0.3704064601	-0.4826090904	0.3470784751
C	-0.7076152396	1.3460524596	2.6176835103
N	1.0985338151	0.3078851897	0.7862684327
C	-1.2584134559	1.7942871152	1.4544454997
C	-1.0488953951	-0.0007570716	3.2072637291
H	-0.0804333529	2.0129881840	3.2058143736
C	-2.3090801996	0.9858281654	0.7013372312
H	-1.0088405220	2.7891372570	1.0927957764
H	0.2952836502	1.0860625042	1.4502398155
C	-1.8024232345	0.0756262506	-0.4541739068
C	-3.0703367745	0.1158697834	1.7207702024
H	-2.9819782425	1.7162924211	0.2431064254
C	-0.9049530641	-1.1112847945	0.0370619950
H	-2.6868237352	-0.3671467521	-0.9181804160
H	-1.2848080522	0.6436548402	-1.2296473737
C	-1.4726987025	-1.7994233011	1.3200479760
H	-0.7787093193	-1.8492870215	-0.7580510348
H	-3.8630389310	-0.4411756417	1.2144429824
C	-2.0643625503	-0.8383054701	2.3821484090
H	-3.5534825187	0.7465208781	2.4714795324
H	-0.7114772415	-2.4498665814	1.7571233457
H	-2.2791635806	-2.4533974651	0.9766026108

H	-1.4799716439	0.2018896752	4.1951494033
H	-0.1292055622	-0.5583972036	3.4158275515
H	-2.5897996075	-1.4797593306	3.0935944538

3

C	0.3980957109	-0.7152841209	1.0541488111
C	0.1174130598	-0.2493737766	2.4649009263
N	1.6057707301	-0.9659838012	0.7050583407
C	-0.5778404770	1.1327335085	2.4059621670
C	-0.8350081536	-1.2660806181	3.1400890805
H	1.0602840023	-0.1828062354	3.0128984948
C	-1.8846873829	1.0294536961	1.5828404527
H	-0.7973944438	1.4820350490	3.4204288156
H	0.0895220470	1.8689110805	1.9448673466
C	-1.5437837472	0.5461688135	0.1521363186
C	-2.7773977432	-0.0045976908	2.2369887852
H	-2.3981334363	1.9890719987	1.5535504254
C	-0.8507894231	-0.8376881948	0.2057363826
H	-2.4566480712	0.4765503439	-0.4490563935
H	-0.8886305569	1.2762694392	-0.3349817489
C	-1.8014658421	-1.8524208545	0.8865880980
H	-0.5814725049	-1.1735609540	-0.7943544687
C	-2.1424625415	-1.3746542005	2.3187454813
H	-1.3321629890	-2.8410358098	0.9263058475
H	-2.7185972679	-1.9499720195	0.2956723889
H	-1.0581001142	-0.9443136214	4.1630073853
H	-0.3536158265	-2.2479380437	3.2027318368
H	-2.8421003892	-2.0634619301	2.7981485337
N	1.7872318277	-1.4112507161	-0.6062336846
C	3.0428135494	-1.5617167890	-0.8944815154
N	3.3871538102	-2.1546736383	-2.0992527043
N	4.0995199009	-1.1748239044	-0.1013773194
H	2.5846761062	-2.2998163734	-2.6968184585
H	4.1679211630	-1.7275040728	-2.5795148492
H	3.7921917248	-0.9200944595	0.8305178476
H	4.9165001822	-1.7671307387	-0.1361843836
N	-3.9602917005	0.1668602989	2.7002373473
N	-4.4774345264	1.4610594593	2.6050643185
C	-5.7043220013	1.5205076088	3.0202223547
N	-6.3102948625	2.7614370393	3.1448020923
N	-6.4915297474	0.4406906277	3.3519135931
H	-5.7409001523	3.5046609064	2.7632068669
H	-7.2724102901	2.8004804856	2.8355584659
H	-5.9467365314	-0.4119380234	3.4177016969
H	-7.1484040923	0.5890422313	4.1042420245

3H⁺

C	0.4100951777	-0.6819727439	1.0319570468
C	0.1040230758	-0.2195531627	2.4394504905
N	1.6175552442	-0.9463785704	0.6977725136
C	-0.5923997814	1.1584607376	2.3797057172

C	-0.8548407015	-1.2369467117	3.0986642801
H	1.0344147836	-0.1471301736	3.0055356615
C	-1.8866964919	1.0514750466	1.5257623119
H	-0.8293121824	1.5073133481	3.3906395910
H	0.0685641689	1.9009947850	1.9241055398
C	-1.5250379399	0.5701704131	0.0927881805
C	-2.7786742173	0.0127104994	2.1646318174
H	-2.3557171999	2.0396180694	1.4625149439
C	-0.8258865529	-0.8045925863	0.1616387522
H	-2.4274664383	0.5020994743	-0.5244975073
H	-0.8687052470	1.3117914838	-0.3708600741
C	-1.7868830598	-1.8218957043	0.8147737194
H	-0.5358175698	-1.1328424112	-0.8350614987
C	-2.1476879141	-1.3546398664	2.2493894750
H	-1.3194304459	-2.8086382894	0.8689554144
H	-2.6951568075	-1.9264305190	0.2114911308
H	-1.0988362618	-0.9257211854	4.1200271858
H	-0.3804013618	-2.2198173119	3.1629028017
H	-2.8534024656	-2.0452292602	2.7154855173
N	1.8136014682	-1.3892389750	-0.5995350987
C	3.0784303134	-1.5989079772	-0.8567532005
N	3.4098205993	-2.1877543369	-2.0524548732
N	4.1184358332	-1.2746638094	-0.0307989902
H	2.6338218529	-2.2884180329	-2.6903531216
H	4.2755581095	-1.8990784392	-2.4841763236
H	3.8258717941	-1.0062793820	0.8993945032
H	4.9547585340	-1.8353653317	-0.0899269918
N	-3.9639613303	0.1503411533	2.6420669107
N	-4.5592139385	1.4098521909	2.5848820732
C	-5.7853421509	1.5415235653	3.1020003426
N	-6.3931762797	2.7385904374	3.0875597661
N	-6.3786121584	0.4721863223	3.6242054022
H	-5.9459661790	3.5534856675	2.6994255484
H	-7.3285417499	2.8530906194	3.4433580941
H	-5.8599857350	-0.3974060412	3.6080695566
H	-7.2870685827	0.5172911730	4.0556299426
H	-4.0902602114	2.2043298356	2.1651394493

3H₂²⁺

C	-1.7259425027	0.2178798775	0.1953818265
C	-0.8107230620	0.9896888475	1.1202940481
N	-2.9835498105	0.2756839833	0.4328166876
C	0.1659513559	-0.0027507003	1.7957275058
C	0.0006658048	2.0106084996	0.2882157400
H	-1.4095430281	1.4996091884	1.8760988398
C	0.9789953401	-0.7568532681	0.7107747435
H	0.8307191597	0.5458978519	2.4683776441
H	-0.3788985186	-0.7300979700	2.4040823843
C	-0.0005502437	-1.5231833600	-0.2179833833
C	1.7258992730	0.2626257167	-0.1263304433
H	1.6415082511	-1.4796573223	1.1946669289

C	-0.9795228356	-0.5264258696	-0.8940819446
H	0.5442615005	-2.0677151422	-0.9941317782
H	-0.5456713106	-2.2634669309	0.3741026497
C	-0.1661037749	0.5015304750	-1.7239288034
H	-1.6424985824	-1.0839950157	-1.5612577987
C	0.8113396754	1.2637255485	-0.7972226948
H	-0.8306008728	1.2173763676	-2.2152518264
H	0.3781718970	-0.0260491887	-2.5122349914
H	0.6658836923	2.5722922234	0.9497403983
H	-0.6639534986	2.7360512992	-0.1888810588
H	1.4105839914	1.9648940256	-1.3795481564
N	-3.8739724543	-0.4095092496	-0.3752904643
C	-5.1865442771	-0.3228039716	-0.0760637962
N	-6.0779318035	-0.9710856729	-0.8325322402
N	-5.5600564389	0.4044282979	0.9680780748
H	-5.8017952266	-1.5291212238	-1.6254467830
H	-7.0661978166	-0.9182044672	-0.6364128672
H	-4.8408374215	0.8767235890	1.5000650862
H	-6.5267526425	0.4983082160	1.2389267416
N	2.9835464253	0.3837522115	-0.3384619953
N	3.8736417243	-0.5009529201	0.2450637509
C	5.1861876350	-0.3349573129	-0.0186122188
N	6.0772600003	-1.1696423200	0.5258057072
N	5.5600435150	0.6551540187	-0.8176942838
H	5.8009600264	-1.9265089024	1.1317592656
H	7.0655305932	-1.0645415048	0.3520160482
H	4.8410689462	1.2578291908	-1.1961167847
H	6.5267499091	0.8203259726	-1.0519392383
H	3.5733869537	-1.2437943580	0.8653230045
H	-3.5740560749	-0.9483326540	-1.1792932227

3aH⁺

C	0.5342578290	-0.7762316102	1.1094506170
C	0.5430984368	-0.5575320659	2.6028214825
N	1.6612524625	-1.0062505993	0.5377805649
C	-0.0537862041	0.8419006492	2.9009484419
C	-0.3435806633	-1.6466645858	3.2594432722
H	1.5695931491	-0.6243484835	2.9681731243
C	-1.4867012042	0.9306125725	2.3305191755
H	-0.0601435186	1.0053988182	3.9818493395
H	0.5709767579	1.6253132691	2.4600044998
C	-1.4369633095	0.7039874359	0.8026475592
C	-2.3218932893	-0.1715942137	2.9476997046
H	-1.9309061439	1.8999975831	2.5527955551
C	-0.8454662125	-0.7001480470	0.4960099022
H	-2.4400299371	0.7656485548	0.3720125862
H	-0.8321121663	1.4857978916	0.3320284995
C	-1.7283283281	-1.7914041385	1.1620570421
H	-0.8423709551	-0.8548717333	-0.5880772530
C	-1.7768169921	-1.5587160874	2.6893441884
H	-1.3318870910	-2.7894290459	0.9494187071

H	-2.7337214789	-1.7420387866	0.7350266662
H	-0.3528449345	-1.4962042676	4.3422574491
H	0.0732488298	-2.6417250223	3.0741160041
H	-2.4284302646	-2.2939986714	3.1636287009
N	1.6789684987	-1.2214510553	-0.8380124932
C	2.8618160081	-1.4721728698	-1.4130952907
N	2.9292875089	-1.6847706004	-2.7360728737
N	3.9505818988	-1.5038095437	-0.6513971264
H	2.1077198596	-1.6599030081	-3.3186254510
H	3.8056503130	-1.8936879522	-3.1870561226
H	3.8290255156	-1.3325719099	0.3390626398
H	4.8682975198	-1.6709694863	-1.0305255486
N	-3.3997502563	-0.0610038601	3.6267746668
N	-3.8287546962	1.2664886729	3.8117997107
C	-4.9084346190	1.4802292572	4.3687928026
N	-6.0053992274	1.8287325348	4.7529603125
H	-6.1986813736	2.0039962588	5.7323634186
H	0.8312842779	-1.2082618537	-1.3932914741

3bH⁺

C	0.3887834207	-0.6808761498	1.0453948090
C	0.1484401580	-0.2583999921	2.4737979344
N	1.5984873479	-0.9392464485	0.6989336015
C	-0.5209387383	1.1395807293	2.4713172025
C	-0.8051861587	-1.2912945512	3.1283863280
H	1.1032726781	-0.2236583902	3.0019253364
C	-1.8453089104	1.0817887440	1.6736877544
H	-0.7110477772	1.4456572022	3.5031185486
H	0.1524847585	1.8820193921	2.0301053658
C	-1.5380640004	0.6511573394	0.2209065477
C	-2.7474637429	0.0412660482	2.3204779233
H	-2.3003573931	2.0737512766	1.6674594695
C	-0.8738451729	-0.7529933540	0.2175042601
H	-2.4565171038	0.6035483947	-0.3709108263
H	-0.8799463518	1.3846960230	-0.2569821652
C	-1.8270376215	-1.7828005628	0.8846121937
H	-0.6890234542	-1.0526384873	-0.8195924458
C	-2.1291805315	-1.3421593596	2.3335993844
H	-1.3758118890	-2.7805453670	0.8765705987
H	-2.7500899580	-1.8374228319	0.3006831645
H	-0.9954295714	-0.9959373540	4.1635229009
H	-0.3338953864	-2.2795183090	3.1528185070
H	-2.8303148180	-2.0349792826	2.8011566502
N	1.8442946817	-1.3450175680	-0.6110470366
C	3.1099150269	-1.6194287442	-0.9492405658
N	3.3964883225	-2.0188775069	-2.1979117667
N	4.0616636190	-1.4867195692	-0.0308183327
H	2.6790193600	-2.1257438870	-2.8969145186
H	4.3417133768	-2.2321106884	-2.4735901320
H	3.7759028372	-1.1843799615	0.8922915134
H	5.0296089962	-1.6835840500	-0.2259513905

N	-3.8872140947	0.2059012851	2.8717840563
N	-4.4494275009	1.4540796204	2.9681492866
H	-5.4389397987	1.3717187116	3.1532598737
H	-4.2601554108	2.1072836086	2.2130908631
H	1.0988928011	-1.4412089599	-1.2908968932

3cH⁺

C	0.3756931489	-0.5981145408	1.0268095368
C	0.0707805100	-0.1493290315	2.4299003379
N	1.5818831706	-0.8962739590	0.6928525058
C	-0.6400887144	1.2251206903	2.4073069452
C	-0.8067058515	-1.2548108126	3.1016216566
H	0.9978416131	-0.0586030310	2.9964063586
C	-1.8880023878	1.2419013252	1.4828735873
H	-0.9142745796	1.5445218619	3.4159915150
H	0.0671091135	1.9617070175	2.0187244310
C	-1.5855579932	0.6334269854	0.0861826438
C	-2.9741088151	0.4860338134	2.1154710657
H	-2.2386707627	2.2707814675	1.3636098862
C	-0.8547866504	-0.7276119636	0.1615471946
H	-2.5077106165	0.5519921307	-0.4950706384
H	-0.9348100985	1.3328452390	-0.4439779906
C	-1.7391470818	-1.8523421295	0.7786199421
H	-0.5632942811	-1.0327025594	-0.8415697174
C	-1.8518001861	-1.8117260784	2.2380814989
H	-1.2262748119	-2.8186188692	0.5914089011
H	-2.7242205753	-1.9687529199	0.3157843268
H	-1.2151825069	-0.9886253456	4.0815945424
H	-0.1512751725	-2.1266679843	3.2969307634
H	-2.6589205729	-2.3687441053	2.7067826590
N	1.7699099269	-1.3404280213	-0.5821343248
C	3.0400061413	-1.6339990265	-0.8248177133
N	3.3612240635	-1.9940193902	-2.0918331327
N	4.0284775291	-1.6042264885	0.0997223975
H	2.5953051431	-2.1078894013	-2.7371595624
H	4.2024954619	-2.5158541845	-2.2777657523
H	3.7783196748	-1.2035129396	0.9920946296
H	4.9914274581	-1.5418923296	-0.1895920684
N	-3.7670022970	-0.2001064195	2.6088415751

4-„in-in“

C	1.2359566144	-0.6362754560	-0.1744396671
C	1.3021083441	-2.0114337424	-0.7984873072
N	2.1824395914	0.1983165843	-0.3959477525
C	1.3311965604	-3.0649655621	0.3371600776
C	0.0374702705	-2.2272274788	-1.6622830256
H	2.2043289190	-2.0797030274	-1.4104861281
C	0.0752475406	-2.9134035262	1.2178526672
H	1.3723645657	-4.0710284789	-0.0966597596
H	2.2365285197	-2.9349226008	0.9396691529
C	0.0462573966	-1.4996481551	1.8316149663

C	-1.1845440394	-3.1272124425	0.3548747305
H	0.0995930128	-3.6571852302	2.0219579780
C	0.0105784467	-0.4263251932	0.7012108469
H	-0.8337952555	-1.3760290319	2.4710984862
H	0.9304822086	-1.3344802052	2.4560498241
C	-1.2210877848	-0.7003411073	-0.1483962052
H	-0.0119196435	0.5816677596	1.1008612229
H	-2.0865613769	-3.0416684034	0.9700600769
C	-1.2230835206	-2.0733958251	-0.7804816082
H	-1.1816310580	-4.1344123819	-0.0784049047
N	-2.2267052371	0.0728807325	-0.3264941226
H	0.0585890970	-3.2291069554	-2.1068077123
H	0.0139875596	-1.5041924632	-2.4834956121
H	-2.1301889404	-2.1868942623	-1.3783755392
N	2.0726652535	1.4423116639	0.2237468991
C	3.0956557415	2.1975487440	-0.0313022003
N	3.0685042508	3.5209037536	0.3806716910
N	4.2428565239	1.8040942632	-0.6839577977
H	2.2665024669	3.7204651476	0.9630926822
H	3.9369074036	3.8664152496	0.7670803408
H	4.1336441957	0.8914101402	-1.1113157322
H	4.6773104865	2.5019720513	-1.2702132861
N	-2.1931437555	1.3005678275	0.3325087144
C	-3.1861555174	2.0589711385	-0.0142811092
N	-3.3959767729	3.2444179567	0.6737594926
N	-4.0765281506	1.7997446816	-1.0323639989
H	-3.6455808926	4.0343503054	0.0935316653
H	-3.9874200899	0.8483863922	-1.3714184606
H	-5.0244033983	2.1111840828	-0.8767394437
H	-2.6407275360	3.4486540549	1.3142908580

4-„in-out“

C	1.0700965019	1.9031590382	-1.0011398519
C	-0.3073183478	1.7639635182	-1.6919276282
C	-1.4113866823	1.5472462316	-0.6306220032
C	-1.0700969491	0.3079524732	0.1700731544
C	0.2780815421	0.3865953383	0.8617124752
C	1.3375510841	0.6536806730	-0.1948348625
C	0.2530983497	1.6097106704	1.8267949783
C	-0.0578958821	2.8930206474	1.0323633400
C	-1.4296945126	2.7536438948	0.3425770721
C	1.0338813644	3.1133942827	-0.0328896365
N	-1.7894639414	-0.7379544127	0.3403398166
N	-3.0399643994	-0.7359893379	-0.2800344303
C	-3.6535500757	-1.8680006605	-0.1188511170
N	-3.1040764277	-3.0053932704	0.4269433854
N	2.3882541152	-0.0403165876	-0.4302014279
N	2.5851999136	-1.1601089801	0.3784869388
C	3.5972365433	-1.8678325231	-0.0173678501
N	4.3013191984	-1.6774373069	-1.1850051849
N	-4.9742304004	-1.9783614845	-0.5248983125

N	4.0301808446	-2.9195313433	0.7756238576
H	-2.3836933164	1.4175460105	-1.1032911525
H	-1.6669349932	3.6670664079	-0.2156579971
H	-2.2195745292	2.6175569347	1.0886056948
H	-0.0781701538	3.7479628723	1.7173275137
H	1.2209380230	1.6939347774	2.3320978620
H	-0.5061208354	1.4413485236	2.5981874909
H	0.4876598123	-0.5392478329	1.3909255986
H	2.0121289067	3.2362302120	0.4440179666
H	0.8320472774	4.0298281568	-0.5998251481
H	-0.5251654631	2.6716179817	-2.2671258453
H	-0.2922480080	0.9272237675	-2.3970142128
H	1.8634717459	2.0255335011	-1.7421552993
H	-5.2866567370	-1.1629993527	-1.0344088268
H	-5.2092173286	-2.8479681719	-0.9845130201
H	-2.2060349877	-2.8161037607	0.8583517267
H	-3.7299872400	-3.5818780088	0.9702844498
H	4.2827839445	-3.7587485312	0.2708733019
H	4.0619079939	-0.7965148945	-1.6259095868
H	5.2895075690	-1.8802135764	-1.1415937349
H	3.4019224809	-3.0964078771	1.5477905055

4-„out-out“

C	1.2462424808	1.3887353047	-0.8445503319
C	-0.0389038878	1.2785209860	-1.7000406850
C	-1.2937447939	1.4066699686	-0.8029898238
C	-1.2418173538	0.3116509549	0.2415581438
C	0.0007993324	0.3746970399	1.1095878807
C	1.2136675791	0.2950538852	0.2020504816
C	0.0214146030	1.7521737072	1.8341631890
C	0.0125959950	2.8821892861	0.7865740857
C	-1.2621388520	2.7732088476	-0.0734704131
C	1.2571143577	2.7554884690	-0.1146109065
N	-2.1025370555	-0.6117085126	0.4572166739
N	-3.2385294534	-0.5973865710	-0.3541832183
C	-3.9825615457	-1.6414031195	-0.1550004791
N	-3.6404714465	-2.7340258759	0.6083966017
N	2.0689321997	-0.6394226782	0.3903919972
N	3.1626904175	-0.6571260192	-0.4771805467
C	4.0015762026	-1.5983028904	-0.1709066342
N	3.9465157237	-2.3843923384	0.9577915139
N	-5.2319367762	-1.6984477310	-0.7528213257
N	5.0589682127	-1.8582849717	-1.0281845879
H	-2.2031535772	1.3035392861	-1.3928007303
H	-1.2881180877	3.5807195080	-0.8147177106
H	-2.1541139257	2.8821100699	0.5524419087
H	0.0278763572	3.8515463045	1.2970432851
H	0.9152655917	1.8167106704	2.4638855573
H	-0.8511739956	1.8286932734	2.4917034058
H	0.0063717154	-0.4530942982	1.8188518371
H	2.1702850803	2.8523171312	0.4821910991

H	1.2701855006	3.5627085606	-0.8565286161
H	-0.0456200569	2.0774495875	-2.4508398097
H	-0.0540827484	0.3259606383	-2.2377084046
H	2.1342005331	1.2729926616	-1.4638875906
H	-5.3808471556	-0.9361942878	-1.4000186849
H	-5.4816088224	-2.5998193094	-1.1374629791
H	-2.8054851370	-2.5601104670	1.1567208688
H	-4.3974040318	-3.1793032820	1.1065486394
H	5.9432952062	-2.0444759239	-0.5744203975
H	3.0644532625	-2.2737929689	1.4453685039
H	4.2571440822	-3.3385444206	0.8455268083
H	5.1281992697	-1.1743784754	-1.7694346052

4H⁺-„in-in“

C	-0.8366676765	-1.1624556955	-0.0456830189
C	-2.0776284135	-1.2538591602	-0.9042610660
N	0.2289479839	-1.8205530258	-0.3191058976
C	-3.3550843608	-1.3344119384	-0.0359386233
C	-2.1307855365	0.0639988416	-1.7335509087
H	-1.9971115743	-2.1132482545	-1.5722396311
C	-3.4379605137	-0.1080625222	0.8958159028
H	-4.2297010292	-1.3768447556	-0.6921625997
H	-3.3551362637	-2.2553953374	0.5551752910
C	-2.2077295002	-0.0996165205	1.8094337547
C	-3.4501254444	1.2046539589	0.0885978484
H	-4.3446419408	-0.1710246736	1.5039186539
C	-0.9122841444	-0.0221591854	0.9664292023
H	-2.2381920496	0.7507205467	2.4979743249
H	-2.1679887533	-1.0054642424	2.4216184695
C	-0.9134630440	1.1798094577	0.0427341299
H	-0.0488464356	-0.0330940635	1.6251068217
H	-3.5182962395	2.0622090195	0.7653392705
C	-2.1757222767	1.3003603612	-0.7776523961
H	-4.3247915979	1.2472144286	-0.5672319869
N	0.1171680425	1.8778732119	-0.2789714511
H	-3.0312117550	0.0657561977	-2.3552909628
H	-1.2658757122	0.1315451247	-2.3984349033
H	-2.1519686630	2.2228654559	-1.3606306797
N	1.3674729050	-1.4276508206	0.3972139076
C	2.4318721319	-2.1126289885	0.0762826642
N	3.6144380828	-1.7571769837	0.7282234553
N	2.4893161366	-3.0465371520	-0.8965492559
H	3.4756477670	-1.5896231917	1.7173620379
H	4.4076290725	-2.3621058715	0.5592656440
H	1.6054713653	-3.2739679787	-1.3329461785
H	3.2263405887	-3.7318578500	-0.9247422184
N	1.3360819962	1.4301263541	0.2482889675
C	2.4261109664	2.1498673282	-0.0188826317
H	1.4529254923	0.4109719471	0.4539870037
N	3.6351580451	1.5891650128	0.1510934427
N	2.2988840872	3.4181663271	-0.4203183110

H	3.7293276497	0.5939870982	0.3283325777
H	4.4728328552	2.1468624175	0.1209143478
H	1.3604933913	3.7360196265	-0.6269975063
H	3.0791343652	3.9225984957	-0.8088274913

4H⁺ - „in-out“

C	1.1070570976	1.8714327035	-1.0357910860
C	-0.2988631574	1.7968690298	-1.6740317508
C	-1.3691417477	1.6432262418	-0.5586941440
C	-1.0468182085	0.3908129322	0.2248859594
C	0.3113100936	0.4176556128	0.8812089592
C	1.3381280525	0.6132600943	-0.2333797871
C	0.3868108778	1.6493511839	1.8307661504
C	0.1172933506	2.9363879000	1.0308243747
C	-1.2895772611	2.8568530014	0.4083918252
C	1.1711374377	3.0912023330	-0.0835846786
N	-1.7556325862	-0.6692560333	0.3834909230
N	-3.0047844107	-0.7331915108	-0.2313165781
C	-3.6914954804	-1.8742821633	-0.1133968045
N	-3.1312414782	-2.8944168744	0.5301541495
N	2.3294068776	-0.1543585299	-0.4852881854
N	2.4766074425	-1.2770233869	0.3094927074
C	3.5315837183	-1.9737720498	-0.0321495920
N	4.3065380978	-1.7449650962	-1.1331678674
N	-4.9223690307	-1.9747642105	-0.6416594083
N	3.9008968338	-3.0256641340	0.7669233718
H	-2.3639630048	1.6155150842	-1.0164450163
H	-1.5142264624	3.7664204081	-0.1571440822
H	-2.0498931154	2.7683219764	1.1914614048
H	0.1617691335	3.7981637006	1.7031634593
H	1.3790367653	1.6747506565	2.2886827854
H	-0.3419921394	1.5353903182	2.6403826557
H	0.5007715509	-0.5152624795	1.4064975941
H	2.1717615045	3.1681000185	0.3510986384
H	0.9935465200	4.0125125554	-0.6486791777
H	-0.5100219308	2.7113519967	-2.2373169739
H	-0.3523151503	0.9591574701	-2.3758442048
H	1.8694251187	1.9460193961	-1.8129695029
H	-5.3672810604	-1.1926660231	-1.0943310226
H	-5.4113552975	-2.8552497989	-0.6573361060
H	-2.2041203236	-2.7429523650	0.9100889455
H	-3.6387469886	-3.7373564211	0.7432452799
H	4.3325763048	-3.8227977443	0.3237152595
H	4.1045321528	-0.8681600153	-1.5952947141
H	5.2785523468	-2.0104565790	-1.0878600663
H	3.2461972395	-3.2437009978	1.5028403453
H	-3.3689136827	0.0306847997	-0.7892300395

4H⁺ - „out-out“

C	1.2990638514	1.3967636425	-0.8358508858
C	0.0195353023	1.3136359535	-1.6972095369

C	-1.2358667647	1.4577289360	-0.7929469479
C	-1.1992370660	0.3577347471	0.2430899464
C	0.0324442724	0.3978355037	1.1172803592
C	1.2375101271	0.2887928580	0.1936101304
C	0.0775067242	1.7714935577	1.8476162035
C	0.0954863467	2.9025425542	0.8037824481
C	-1.1845970493	2.8215370079	-0.0488894750
C	1.3359305935	2.7584381225	-0.1004503935
N	-2.0480046691	-0.5819555911	0.4598026186
N	-3.1799882064	-0.6520684188	-0.3506364662
C	-4.0284041075	-1.6641991740	-0.1430531137
N	-3.7358951378	-2.5637808802	0.7916974680
N	2.0521218461	-0.6842138672	0.3583950090
N	3.1302254037	-0.7323377263	-0.5061574914
C	3.9788079279	-1.6731779416	-0.1796795717
N	3.9339936469	-2.4127144892	0.9680998857
N	-5.1523180267	-1.7576599236	-0.8722858608
N	5.0094525586	-1.9466627965	-1.0441733505
H	-2.1344465019	1.4258308018	-1.4187502892
H	-1.2040782762	3.6234760303	-0.7932924748
H	-2.0722076225	2.9443544515	0.5806170844
H	0.1228005586	3.8690092154	1.3154347876
H	0.9747606135	1.8029074706	2.4716129367
H	-0.7869735832	1.8682541756	2.5130016586
H	0.0224098567	-0.4352606926	1.8197118436
H	2.2489079176	2.8328904462	0.4970040380
H	1.3659340526	3.5716123553	-0.8337129320
H	0.0081968576	2.1213742540	-2.4358587077
H	-0.0079280206	0.3674890504	-2.2454201338
H	2.1831185401	1.2617002030	-1.4565326681
H	-5.3922980477	-1.0644639183	-1.5625720849
H	-5.7585864576	-2.5581597753	-0.7936919583
H	-2.8762437153	-2.4260469338	1.3093645319
H	-4.3759805923	-3.2965539006	1.0501449741
H	5.8904639981	-2.2258447669	-0.6374975054
H	3.0765731488	-2.3008466412	1.4918621995
H	4.3329774104	-3.3386095520	0.9492427723
H	5.0896976431	-1.2906804394	-1.8076303164
H	-3.3410803531	0.0074500914	-1.1031827316

4H₂²⁺ „in-in“

C	-1.2397325486	0.6148746956	-0.1781368619
C	-1.2594584485	2.0065898117	-0.7608411605
N	-2.2702387075	-0.1172608299	-0.3804688139
C	-1.2589433412	3.0086912265	0.4251124183
C	-0.0000786268	2.2128715211	-1.6281224984
H	-2.1641405325	2.1240877199	-1.3583875315
C	-0.0000987372	2.7933523410	1.2846574282
H	-1.2812425028	4.0267160803	0.0272728324
H	-2.1650318817	2.8814977435	1.0249411017
C	-0.0000459481	1.3605959423	1.8529380988

C	1.2587296378	3.0087825150	0.4251117836
H	-0.0001241121	3.4972430801	2.1208453709
C	-0.0000102054	0.3260720630	0.6692259346
H	0.8814085217	1.1886955956	2.4775383876
H	-0.8814862883	1.1886318395	2.4775408565
C	1.2396895349	0.6149632166	-0.1781403938
H	0.0000268854	-0.6976274231	1.0545269883
H	2.1648276123	2.8816546689	1.0249401361
C	1.2593164255	2.0066811032	-0.7608413710
H	1.2809548489	4.0268090014	0.0272722540
N	2.2702459431	-0.1170997677	-0.3804779512
H	-0.0001154313	3.2283399377	-2.0324494530
H	-0.0000537672	1.5278460471	-2.4809487328
H	2.1639895030	2.1242440536	-1.3583885694
N	-2.3882521865	-1.3788116182	0.1876756998
C	-3.5333644119	-2.0530741009	-0.0830650806
N	-3.7669542034	-3.2202943578	0.5248228811
N	-4.3824229449	-1.5440000260	-0.9608747905
H	-3.1038126228	-3.6357939871	1.1596116800
H	-4.6195931292	-3.7343449928	0.3588881264
H	-4.1737384480	-0.6313296742	-1.3468025251
H	-5.2259713034	-2.0242676703	-1.2358709761
N	2.3883495230	-1.3786453330	0.1876575462
C	3.5335217811	-2.0528125880	-0.0830676068
H	1.8551782704	-1.6471999825	1.0065934894
N	3.7671823138	-3.2200290252	0.5248011750
N	4.3825772366	-1.5436416709	-0.9608234066
H	3.1039940567	-3.6356567419	1.1594574116
H	4.6198624023	-3.7340143236	0.3588752584
H	4.1738400796	-0.6309722088	-1.3467249690
H	5.2261503747	-2.0238557116	-1.2358373829
H	-1.8550686213	-1.6473181700	1.0066192162

4H₂²⁺ „in-out“

C	-1.3372365880	0.5732078810	-0.2173363488
C	-1.1088714392	1.8907595728	-0.9167528251
N	-2.4255153019	-0.0545978692	-0.4632041834
C	-1.0937064993	3.0052372875	0.1646481400
C	0.2542767914	1.8479194428	-1.6412693335
H	-1.9135698615	2.0605856952	-1.6331013708
C	0.0219950866	2.7184798643	1.1857387963
H	-0.9324342692	3.9711612784	-0.3219684524
H	-2.0663128819	3.0578723149	0.6618835893
C	-0.2340021733	1.3607752583	1.8641831226
C	1.3868167845	2.6909858894	0.4734586509
H	0.0305626824	3.5000628868	1.9495755525
C	-0.2383666545	0.2287160813	0.7787024201
H	0.5403312886	1.1353442165	2.6027902143
H	-1.1938407069	1.3613640676	2.3882969004
C	1.1089134145	0.2667658928	0.0715908372
H	-0.3541858566	-0.7506602727	1.2473141335

H	2.1927020940	2.5168109562	1.1926709318
C	1.3863520124	1.5809616010	-0.6179798124
H	1.5884821085	3.6520536117	-0.0073036672
N	1.8600342926	-0.7646647785	0.2022760999
H	0.4357754545	2.8085541903	-2.1300180242
H	0.2513528655	1.0835771818	-2.4237646849
H	2.3457168457	1.5881880415	-1.1423978124
N	-2.7249916820	-1.2329803599	0.1960927011
C	-3.9068689743	-1.8215552291	-0.0856161669
N	-4.2572443621	-2.9369734594	0.5635476641
N	-4.6873031741	-1.2829001235	-1.0114830129
H	-3.7014817663	-3.3152261689	1.3146015569
H	-5.1320521834	-3.4006747386	0.3689130178
H	-4.3708523874	-0.4366858961	-1.4672687906
H	-5.5940609666	-1.6629338508	-1.2362310062
N	3.1206116465	-0.7434641761	-0.3704812651
C	3.9515524418	-1.7800981644	-0.1457028973
H	3.4463972626	0.0539382356	-0.9043826782
N	5.1611285624	-1.7846287377	-0.7127957131
N	3.5490620175	-2.7730842548	0.6379261369
H	5.4571273671	-1.0584345155	-1.3471473232
H	5.8254949676	-2.5203902770	-0.5240940210
H	2.6348399146	-2.7053191757	1.0621788603
H	4.1221118259	-3.5844237284	0.8113598985
H	-2.1162719988	-1.6361126713	0.8984861652

4H₂²⁺ - „out-out“

C	-1.2425982880	0.2285780020	0.1141401038
C	-1.2716539337	1.4433416922	-0.7844116404
N	-2.1228693899	-0.6854863804	0.2897804118
C	-1.2604359394	2.7058652888	0.1244657659
C	0.0000939141	1.4248289809	-1.6696779565
H	-2.1480359945	1.4688366158	-1.4378698612
C	0.0000023683	2.6945292439	1.0096945013
H	-1.2798778104	3.5966254672	-0.5096956276
H	-2.1609963670	2.7343683350	0.7445323728
C	-0.0000537410	1.4350029854	1.8934109299
C	1.2605139954	2.7058267103	0.1245694812
H	-0.0000104760	3.5824307148	1.6468887784
C	-0.0000365200	0.1619904164	0.9833649673
H	0.8797811426	1.4084881780	2.5422310055
H	-0.8799431377	1.4085146063	2.5421579593
C	1.2426000605	0.2285393489	0.1142446722
H	-0.0000757451	-0.7525567788	1.5750185707
H	2.1610240102	2.7343037359	0.7447106218
C	1.2717692838	1.4433013961	-0.7843050393
H	1.2800351717	3.5965850234	-0.5095920590
N	2.1228212731	-0.6855611980	0.2899483452
H	0.0001348945	2.3096646714	-2.3116756369
H	0.0001080317	0.5499888133	-2.3263151389
H	2.1482051800	1.4687675948	-1.4376919445

N	-3.3079660266	-0.6287743723	-0.4230287045
C	-4.2449677877	-1.5659115274	-0.1736927744
N	-5.4006749103	-1.5327597155	-0.8438413749
N	-3.9938309340	-2.5011780925	0.7329930630
H	-5.5890450375	-0.8394717781	-1.5514857417
H	-6.1321041032	-2.2028440900	-0.6593395529
H	-3.1095396626	-2.4646559913	1.2219268809
H	-4.6533077885	-3.2340212679	0.9444164252
N	3.3079679844	-0.6289041354	-0.4227808403
C	4.2449399675	-1.5660409024	-0.1733254530
H	3.5104371811	0.1258675952	-1.0680627218
N	5.4006839281	-1.5329553509	-0.8434137005
N	3.9937497360	-2.5012198375	0.7334352666
H	5.5890241893	-0.8398435403	-1.5512387014
H	6.1321136646	-2.2030048268	-0.6587867134
H	3.1094324713	-2.4646460999	1.2223185097
H	4.6531242541	-3.2341681492	0.9448138063
H	-3.5103151092	0.1259506184	-1.0684022556

4aH⁺

C	0.4080876262	0.0416182437	0.6733483355
C	-0.0574088669	0.4482438910	2.0502804701
N	1.6559402580	-0.0844986311	0.4159329607
C	-1.0915644468	1.5968217130	1.9368346804
C	-0.7522592074	-0.7903870053	2.6796680780
H	0.8039886313	0.7478639328	2.6488936726
C	-2.2870300360	1.1471563714	1.0733519986
H	-1.4252853278	1.8707452667	2.9419507073
H	-0.6236791680	2.4856607101	1.5033507951
C	-1.7843023848	0.7941578514	-0.3320183430
C	-2.9653071622	-0.0962589836	1.6781798375
H	-3.0125499358	1.9619637213	1.0021439317
C	-0.7375314788	-0.3506864266	-0.2501576072
H	-2.6097856568	0.4781434847	-0.9768181441
H	-1.3131085373	1.6571118202	-0.8107542981
C	-1.3274501708	-1.5696422378	0.4427856400
H	-0.3664731936	-0.5607235010	-1.2516930280
H	-3.8190303219	-0.3991394092	1.0640916559
C	-1.9424250188	-1.2496143425	1.7838719028
H	-3.3537599798	0.1223777069	2.6770542037
N	-1.1728914701	-2.7995396529	0.1088620636
H	-1.1335484738	-0.5260521680	3.6701271477
H	-0.0365329339	-1.6066011390	2.8094394081
H	-2.3974300363	-2.1508382409	2.1981622305
N	1.9280855357	-0.5382236756	-0.8851456368
C	2.6496514748	-1.4582613975	-1.2167065815
N	3.1437032528	-2.4724485088	-1.7160420861
H	1.7248036381	-3.9737731920	-2.1420448369
H	4.1377785329	-2.4742038817	-1.9308776527
N	-0.3562656535	-3.0716631958	-0.9832183397
C	-0.1108723350	-4.3517395139	-1.3075338437

H	0.2347797774	-2.3522897069	-1.3862104643
N	0.9366017484	-4.6241170571	-2.0920272615
N	-0.9391025534	-5.2983460828	-0.8689519019
H	1.0611341129	-5.5485240232	-2.4741848881
H	-1.6952632726	-5.0162424640	-0.2593127714
H	-0.6908749662	-6.2735222757	-0.9186260349

4bH⁺

C	0.3312785018	-0.1382121493	0.5198411655
C	-0.0169275000	0.3187582645	1.9214292218
N	1.5312758358	-0.4231561798	0.2009366006
C	-0.9712947651	1.5350777608	1.8722794121
C	-0.7526884591	-0.8606344976	2.6155858748
H	0.9033176760	0.5578605478	2.4560094758
C	-2.2555790107	1.1680106444	1.1012193088
H	-1.2134719752	1.8392115142	2.8949209028
H	-0.4771051712	2.3873337563	1.3957574619
C	-1.8818042627	0.7763933676	-0.3341107174
C	-2.9743293271	-0.0272601799	1.7558368188
H	-2.9278198331	2.0299361538	1.0769291166
C	-0.9111274818	-0.4308278441	-0.3204572850
H	-2.7729850436	0.5142125993	-0.9125963306
H	-1.3958200755	1.6081892797	-0.8527064240
C	-1.4942466890	-1.6090428376	0.4378283655
H	-0.6619979133	-0.7062492905	-1.3423008337
H	-3.8869991736	-0.2692482078	1.2021680995
C	-2.0287872696	-1.2467494604	1.8011095873
H	-3.2781833283	0.2171805887	2.7777540159
N	-1.3301790328	-2.8471773976	0.1401618872
H	-1.0559446723	-0.5583823609	3.6222327324
H	-0.0881196349	-1.7228072451	2.7120183702
H	-2.5117080790	-2.1160580001	2.2508335335
N	1.7102764308	-1.0225645510	-1.0981700518
N	-0.5044643832	-3.1223281500	-0.9604220120
C	-0.4385249605	-4.4023428019	-1.3490256935
H	0.2997572885	-2.4975389923	-1.1584017411
N	0.4592435723	-4.7587734491	-2.2810229502
N	-1.2737603626	-5.2909489345	-0.8176325752
H	0.5349698992	-5.7103301696	-2.6017598142
H	-1.8607856282	-4.9747075418	-0.0560093873
H	-1.2761411729	-6.2597082352	-1.0913708135
H	1.5239631720	-0.3297243853	-1.8250900057
H	2.7066441875	-1.2133506192	-1.1557019400
H	1.0460616414	-4.0691919967	-2.7225993757

4cH⁺

C	-0.1194962938	-0.679480183	-0.0599195657
C	0.8662641662	-0.9854676294	1.0514271863
N	-1.4237077972	-0.4742192723	0.3395752408
C	2.0580354106	-1.7599367098	0.4628865414
C	1.3724411302	0.3014604351	1.7478581636

H	0.3541460095	-1.5961301777	1.8001236119
C	2.7103966669	-0.9002326762	-0.6330881397
H	2.7797433160	-1.9852901740	1.2526240529
H	1.7237780209	-2.7174154261	0.0515746973
C	1.6997149941	-0.7011414687	-1.7829300359
C	3.2393076420	0.4153517226	-0.0217013633
H	3.5754162420	-1.4272382490	-1.0435886597
C	0.2880581476	-0.5388888951	-1.3554413886
H	1.9677763730	0.1440460928	-2.4300397509
H	1.7223976423	-1.5706957425	-2.4600159892
C	1.3218243626	2.0335141387	-0.0492983603
H	-0.4473824952	-0.2865132432	-2.1123194192
H	3.6693502325	1.0566106425	-0.7949675056
C	2.1967519413	1.2187872521	0.8046989248
H	4.0557187948	0.1584419728	0.6600122098
N	0.6310858844	2.6684204759	-0.7215049223
H	2.0209933826	0.0032321121	2.5767121987
H	0.5416690231	0.8637004698	2.1811346558
H	2.7434278690	1.9359753553	1.4253619341
N	-2.3052536500	-0.2432958285	-0.5465843268
C	-3.5674095996	-0.0282960611	0.0129260998
N	-4.5066430578	0.2585838640	-0.8755477351
N	-3.7904059216	-0.1133142545	1.3121217870
H	-4.2333579371	0.3146424312	-1.8473690128
H	-5.4656387510	0.4513077457	-0.6279733797
H	-2.9906535825	-0.3304785784	1.8961435297
H	-4.6920249097	0.0463368068	1.7350584269

5-„up-up“

C	0.8412807127	1.1340269024	-0.9025932066
C	1.1781831508	2.6501931824	-0.7561521611
C	0.0545938939	3.3673398838	-1.5158109355
C	-1.0862529012	2.6620973045	-0.7709175587
C	-0.7638570875	1.1425678832	-0.9132905623
C	0.8187796921	2.8951196762	0.7411199071
H	2.2034785067	2.9010928436	-1.0313885564
H	0.0605427935	3.1650148303	-2.5908798588
H	0.0592465725	4.4515837469	-1.3635264975
H	-2.1051293041	2.9243195654	-1.0593670509
C	-0.7439886249	2.9031507144	0.7310702019
H	-1.1706431499	0.6580533607	-1.7959970526
C	-1.2849838952	0.5773650594	0.3870556484
H	1.2547895953	0.6449977950	-1.7797091844
C	-0.7708460113	1.5078108549	1.4457619592
H	-1.2653550874	3.7357667559	1.2024441478
C	0.8224030725	1.4999002105	1.4563024749
H	1.3426211956	3.7223959756	1.2191092954
C	1.3406044053	0.5641664444	0.4044426928
H	1.2902498090	1.3995896723	2.4332797266
H	-1.2522431748	1.4118496020	2.4165901066
N	2.0876492990	-0.4415185025	0.6513246900

N	-2.0428373668	-0.4226065736	0.6243340262
N	-2.4316643235	-1.1617570303	-0.4945675973
C	-3.2260070292	-2.1356176531	-0.1724741162
N	2.5001568125	-1.1729534172	-0.4636507889
C	3.1370244028	-2.2500955632	-0.1224093136
N	-3.5801283122	-3.0587366745	-1.1436914308
N	-3.7723277804	-2.3473778315	1.0734943468
H	-4.5502709181	-3.3438892278	-1.1297169045
H	-3.2576809461	-2.7879828606	-2.0628330446
H	-3.3425353219	-1.7541218616	1.7742612035
H	-3.8876079514	-3.3132567415	1.3443426282
N	3.7595029862	-3.0014582025	-1.1074569277
N	3.2521152891	-2.7415904275	1.1582766239
H	3.6544807768	-4.0025223772	-1.0083083075
H	3.5331475469	-2.6716972888	-2.0360947864
H	2.9357712290	-2.0688535769	1.8475382140
H	4.1243684437	-3.2009934536	1.3764909491

5-„up-down“

C	0.3823887433	1.3838378156	-1.1807259153
C	0.6979349227	2.8621614687	-0.7997818741
C	-0.6193547883	3.6133123168	-1.0313405040
C	-1.4711705831	2.6622251530	-0.1801013814
C	-1.1568908754	1.2456200844	-0.7487120520
C	0.7846133620	2.7513183970	0.7537977454
H	1.5906967401	3.2614609211	-1.2831716508
H	-0.9233809806	3.6441387032	-2.0818641030
H	-0.6020206210	4.6365074796	-0.6422965672
H	-2.5374154817	2.8807854897	-0.1067873447
C	-0.7124061420	2.6140272321	1.1818352079
H	-1.7879733392	0.9220618477	-1.5712669140
C	-1.2574744002	0.3707576486	0.4787894566
H	0.5371139517	1.1268174677	-2.2272737743
C	-0.4872556430	1.1032205152	1.5385245629
H	-1.0977494942	3.2763442828	1.9564610399
C	1.0408115366	1.2465586658	1.1094812541
H	1.3998087697	3.5071557596	1.2412851559
C	1.2519243734	0.6002021220	-0.2325335505
H	1.7732277069	0.9890467102	1.8679124918
H	-0.6618080985	0.7588112082	2.5554950768
N	2.0053267249	-0.3652075861	-0.5931474997
N	-1.8768399767	-0.7278708528	0.6765669068
N	-2.5440954712	-1.2502046579	-0.4332467821
C	-3.1778130946	-2.3436765925	-0.1396581485
N	2.7518163124	-0.9562426570	0.4279958089
C	3.5081520869	-1.9094439509	-0.0219964945
N	-3.7630744395	-3.0724704513	-1.1630113739
N	-3.3349111699	-2.8653648185	1.1245569121
H	-4.6763578279	-3.4513234618	-0.9507826310
H	-3.7306193612	-2.5832389411	-2.0471277183
H	-2.7422635731	-2.3936933990	1.7984820045

H	-3.3341828928	-3.8731411725	1.1874363120
N	4.1974265645	-2.7001997896	0.8839680496
N	3.7037552072	-2.2211090676	-1.3487238052
H	5.1460680323	-2.9279826343	0.6177359786
H	4.1224429745	-2.3509010129	1.8297271785
H	3.0466632817	-1.7333482746	-1.9470723871
H	3.8228339630	-3.2020189684	-1.5565786706

5-„down-down“

C	-0.3045849921	-0.1255768231	0.1800493715
C	0.1618362448	-0.1137165396	1.6672417507
C	1.6878304772	0.0287115680	1.5936197539
C	1.6674844682	1.2623050497	0.6815587268
C	0.7623492467	0.8496305261	-0.5184487771
C	-0.3151665570	1.3034093937	2.1098130568
H	-0.2330101707	-0.9395569726	2.2607913455
H	2.1833455589	-0.8365376245	1.1428464644
H	2.1463141605	0.2245457406	2.5682853436
H	2.6309971322	1.6790798806	0.3848612815
C	0.7228355205	2.2525758156	1.4301179964
H	1.2785858130	0.3673736379	-1.3470147660
C	0.0945670650	2.1461877246	-0.8946793809
H	-0.3341312283	-1.1065414014	-0.2915398260
C	-0.3648664836	2.7375541967	0.4101385138
H	1.2241392339	3.0021412000	2.0418853059
C	-1.4242840458	1.7692050056	1.1040187029
H	-0.5076977851	1.4181430903	3.1762433063
C	-1.6473442788	0.5540547406	0.2453985358
H	-2.3261108568	2.2441773189	1.4768321163
H	-0.6381394025	3.7871940829	0.3704628983
N	-2.7032257063	0.0914790835	-0.3038677961
N	0.0289850780	2.5894830435	-2.0903621928
N	-0.5858358696	3.8341040318	-2.2343513668
C	-0.7468001530	4.1495156573	-3.4820025305
N	-3.8601105780	0.8480856200	-0.1087947575
C	-4.8938463805	0.2950582636	-0.6642713591
N	-1.1873385933	5.4252111488	-3.7994699939
N	-0.5258459944	3.3153709424	-4.5548272445
H	-1.8772215715	5.4650948005	-4.5380285048
H	-1.4591330939	5.9479497543	-2.9777237423
H	-0.0419249168	2.4689358569	-4.2770935175
H	-0.1695746163	3.7580493547	-5.3895013210
N	-6.0895973657	0.9949482324	-0.6971357036
N	-4.9247501276	-0.9568097296	-1.2369954695
H	-6.9144640600	0.4419189370	-0.5062465540
H	-6.0473841163	1.8477036837	-0.1556842213
H	-3.9929744269	-1.3424855437	-1.3401645060
H	-5.5190276282	-1.0544307476	-2.0475009395

5H⁺-„up-up“

C	-0.1363921405	-0.2277842166	0.3430291664
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C	0.2485430036	-0.0786897007	1.8514000079
C	1.7677350535	0.1351364049	1.8233485909
C	1.7277654769	1.2989698845	0.8254542513
C	0.9126087552	0.7531124889	-0.3839692282
C	-0.3134705622	1.3388605174	2.1650787054
H	-0.1302890565	-0.8793185088	2.4875108870
H	2.3259002981	-0.7318833509	1.4600862711
H	2.1669314474	0.4202790941	2.8003503832
H	2.6826603331	1.7389261991	0.5392460291
C	0.7055888811	2.2901222732	1.4585573554
H	1.4877625262	0.2376313872	-1.1474887929
C	0.1770916461	1.9762442591	-0.8844929209
H	-0.0607805676	-1.2513633128	-0.0272346769
C	-0.3509396321	2.6378323567	0.3550578925
H	1.1381444215	3.1065923223	2.0330952878
C	-1.3952830831	1.6651447017	1.0852530460
H	-0.5636604843	1.5188047447	3.2086214625
C	-1.5022247338	0.4081767118	0.2833140539
H	-2.3423237089	2.1120058153	1.3771365372
H	-0.6884408295	3.6637696294	0.2330886822
N	-2.5781909891	0.0754002270	-0.3245545755
N	-0.0082133331	2.4046956451	-2.0725081619
N	0.5013397675	1.6096453750	-3.0897344598
C	0.4548095190	2.2206404600	-4.2462134009
N	-2.5251174749	-1.0654291076	-1.1267178184
C	-3.6405774249	-1.4176536519	-1.7755136271
N	0.7853165242	1.5056118962	-5.3756106747
N	0.1087239921	3.5259826515	-4.4311740445
H	1.2483857936	2.0186676823	-6.1126785219
H	1.2130371861	0.6132903400	-5.1734105432
H	-0.2795077926	3.9726291217	-3.6111385307
H	-0.2651896041	3.8040002792	-5.3249923765
N	-3.6362348648	-2.4943113842	-2.5775032681
N	-4.7410989452	-0.6925123141	-1.5996834920
H	-4.4276061052	-2.7107667315	-3.1618854155
H	-2.8193887882	-3.0761286966	-2.6718792713
H	-4.6673027896	0.1171213603	-0.9956816728
H	-5.6367495878	-0.9811115963	-1.9576225363
H	-1.6349361277	-1.4769282565	-1.3857536001

5H⁺ „up-down“

C	0.2925208768	1.4868352502	-1.1968089777
C	0.4634236215	2.9850093854	-0.8014207993
C	-0.9265425307	3.5944347801	-1.0275169298
C	-1.6755913909	2.5566855272	-0.1821915808
C	-1.2251780723	1.1807112307	-0.7583189772
C	0.5572976142	2.8705940652	0.7493365148
H	1.3081785878	3.4802787671	-1.2809586847
H	-1.2313873364	3.6006655552	-2.0769643829
H	-1.0109122592	4.6116102975	-0.6351637487
H	-2.7572807124	2.6646359741	-0.1082399060

C	-0.9163755715	2.5782958314	1.1780246235
H	-1.8133388641	0.7982115613	-1.5868039521
C	-1.2302495742	0.2886736111	0.4624814668
H	0.4751671887	1.2485857136	-2.2425693287
C	-0.5476105986	1.0963483273	1.5285603879
H	-1.3614274393	3.1949306764	1.9562320284
C	0.9648733764	1.3958210752	1.0972958565
H	1.0986174198	3.6718706855	1.2486289200
C	1.2128195438	0.7763620492	-0.2486360951
H	1.7165855623	1.2489923394	1.8734896430
H	-0.6761108990	0.7337543092	2.5456563512
N	1.9871612859	-0.1681322826	-0.6310488003
N	-1.7103056063	-0.8802293198	0.6482744707
N	-2.2778815153	-1.4828430783	-0.4620723958
C	-2.9398399456	-2.5653511493	-0.1447887050
N	2.7674695432	-0.7822802098	0.3472309992
C	3.5479025317	-1.8009260730	-0.0273489671
N	-3.4112829709	-3.3621526590	-1.1613543604
N	-3.2166401610	-2.9762140570	1.1274077035
H	-4.2994403720	-3.8181101465	-1.0073556094
H	-3.3147669295	-2.9474283489	-2.0772726975
H	-2.7268592093	-2.4596272110	1.8451090763
H	-3.3580279839	-3.9608648079	1.2912032001
N	4.3402682570	-2.4046344255	0.8734717992
N	3.5256968011	-2.1922112690	-1.2979656642
H	4.8323979013	-3.2535494148	0.6457007017
H	4.3957025488	-2.0812229858	1.8258222495
H	2.9001890333	-1.6970530418	-1.9219929392
H	4.1797571282	-2.8652501820	-1.6624873556
H	2.6536861205	-0.5550683503	1.3291388650

5H⁺ „down-down“

C	-0.2968661403	-0.1716172611	0.3623331643
C	0.2447137554	-0.0732930347	1.8185251576
C	1.7621001335	0.0815210730	1.6472518073
C	1.6759356467	1.2638880533	0.6743481635
C	0.7157093518	0.7850116893	-0.4534392249
C	-0.2211139765	1.3610769499	2.2074654640
H	-0.1021971668	-0.8681134951	2.4794221349
H	2.2418606525	-0.8014463164	1.2174008224
H	2.2693416322	0.3304471945	2.5833424333
H	2.6159077935	1.6710936898	0.3030005236
C	0.7649198844	2.2839267985	1.4215133957
H	1.1850164426	0.2544440336	-1.2790628495
C	-0.0001630404	2.0466429296	-0.8603266260
H	-0.3462069427	-1.1736360502	-0.0588480931
C	-0.3785408022	2.7092561690	0.4393558040
H	1.2871509272	3.0669381801	1.9675751626
C	-1.3901997508	1.7662881887	1.2413642073
H	-0.3667760255	1.5367426251	3.2715150684
C	-1.6262764687	0.5182406264	0.4395475047

H	-2.2590422891	2.2608878244	1.6762660181
H	-0.6710778054	3.7515676107	0.3641230719
N	-2.6703052113	0.0554786105	-0.1387043223
N	-0.1934025363	2.4136149876	-2.0676797790
N	-0.8841183184	3.6056161618	-2.2324342970
C	-0.9552603518	3.9496881851	-3.4936586716
N	-3.8303545791	0.8255371061	-0.0509692861
C	-4.9298896586	0.3612633222	-0.6541972898
N	-1.4632675982	5.1845972831	-3.8025230922
N	-0.5667090676	3.1702241840	-4.5487088449
H	-1.9571104234	5.2923920044	-4.6753621768
H	-1.8360116075	5.7009722937	-3.0204255527
H	-0.0410737555	2.3525751859	-4.2675133814
H	-0.2349912086	3.6409227351	-5.3772921775
N	-6.0634369643	1.0800693005	-0.6233412994
N	-4.8734883168	-0.8140816553	-1.2731064939
H	-6.8861716935	0.7775538355	-1.1192980160
H	-6.1344749511	1.9275469206	-0.0835749150
H	-3.9782702641	-1.2875367373	-1.2836913641
H	-5.6904870395	-1.2593644473	-1.6573836746
H	-3.7947862658	1.7841022456	0.2789625243

5H₂²⁺ - „up-up“

C	0.8045187863	1.0142063778	-0.9144552650
C	1.1330336179	2.5346953832	-0.7308785894
C	0.0000858925	3.2569606032	-1.4675221001
C	-1.1328722976	2.5347539179	-0.7308368738
C	-0.8044441530	1.0142490347	-0.9144257281
C	0.7808713588	2.7342599155	0.7747643802
H	2.1535981518	2.7975906714	-1.0076379462
H	0.0000617979	3.0935730136	-2.5479325087
H	0.0001171808	4.3337275588	-1.2823386249
H	-2.1534331065	2.7977044293	-1.0075578393
C	-0.7806437281	2.7342998197	0.7747933574
H	-1.1879749595	0.5881872887	-1.8417286734
C	-1.3395705777	0.4355627637	0.3771914909
H	1.1879958980	0.5881274564	-1.8417724820
C	-0.7922746026	1.3191752615	1.4568551737
H	-1.3058012304	3.5448927131	1.2737717105
C	0.7924549298	1.3191343901	1.4568263690
H	1.3060891601	3.5448257452	1.2737232152
C	1.3396683989	0.4354970641	0.3771420170
H	1.2626358203	1.1967285466	2.4284960721
H	-1.2624263628	1.1967931460	2.4285419935
N	2.1978245273	-0.4771232317	0.6290965156
N	-2.1977540126	-0.4770220834	0.6291793732
N	-2.7628409088	-1.1845261993	-0.4207446962
C	-3.7632255903	-2.0428952320	-0.1265746926
N	2.7628444356	-1.1846499123	-0.4208416038
C	3.7631563692	-2.0431115240	-0.1267125962
N	-4.3839820046	-2.6930319209	-1.1161635303

N	-4.0928680784	-2.2312500209	1.1433643085
H	-5.1537631904	-3.3179193627	-0.9285249022
H	-4.1382895480	-2.5542809898	-2.0840091727
H	-3.6088635819	-1.6875042485	1.8463870731
H	-4.8207230278	-2.8721935710	1.4199337196
N	4.3837741324	-2.6933553894	-1.1163208970
N	4.0928535467	-2.2314719965	1.1432119394
H	5.1535911063	-3.3182098283	-0.9287180824
H	4.1382055604	-2.5544130317	-2.0841707059
H	3.6088966877	-1.6877139826	1.8462577581
H	4.8206846185	-2.8724560863	1.4197500284
H	2.5817690134	-0.9383960615	-1.3877868598
H	-2.5819390296	-0.9381334276	-1.3876881251

5H₂²⁺ - „up-down“

C	0.5099284453	1.2633041765	-1.1506572705
C	0.8844461376	2.7205962535	-0.7301197347
C	-0.3785578223	3.5397075295	-1.0177500864
C	-1.3234504985	2.6314015033	-0.2223458738
C	-1.0547089751	1.2026981159	-0.8024201165
C	0.8849696804	2.5876731537	0.8224822287
H	1.8176590165	3.0749471742	-1.1661311213
H	-0.6240774334	3.6079703966	-2.0799370246
H	-0.3280650445	4.5522656486	-0.6102167546
H	-2.3771221078	2.9073976615	-0.1977730916
C	-0.6353081170	2.5185334729	1.1725764365
H	-1.6405119364	0.9720386734	-1.6921791166
C	-1.2834267408	0.3345244473	0.4111837160
H	0.7049669114	1.0133224071	-2.1910463930
C	-0.5049773194	0.9917023752	1.5145481407
H	-1.0256647568	3.1792879953	1.9425617733
C	1.0469205658	1.0614757011	1.1702653001
H	1.5135035722	3.2959130389	1.3568592935
C	1.3138021259	0.4433930484	-0.1746099081
H	1.7044891074	0.7998959447	1.9978648375
H	-0.7478434545	0.6427576120	2.5146635501
N	2.1140527114	-0.4724799158	-0.5682968545
N	-2.0509297675	-0.6632847570	0.6330456896
N	-2.8147881207	-1.1580803670	-0.4121271964
C	-3.7384728195	-2.0997178115	-0.1307400219
N	2.9000104266	-1.1123826452	0.3767182530
C	3.8573634121	-1.9556735671	-0.0600900661
N	-4.5050969951	-2.5827427762	-1.1134516179
N	-3.8564027627	-2.5304217657	1.1183093869
H	-5.2362653691	-3.2521275105	-0.9251424659
H	-4.4073468379	-2.2740552508	-2.0683617749
H	-3.2701913995	-2.1076573326	1.8258828574
H	-4.5146889745	-3.2487874099	1.3780391850
N	4.6445607275	-2.5721495273	0.8269685461
N	3.9872390954	-2.1600782003	-1.3644173484
H	5.4002866555	-3.1704531848	0.5285279158

H	4.5383924108	-2.4366216931	1.8205022195
H	3.3842835004	-1.6433845898	-1.9907735054
H	4.6709410846	-2.7979939166	-1.7418129506
H	2.8540938219	-0.8645248082	1.3591342984
H	-2.7779341556	-0.7466433002	-1.3382103343

5H₂²⁺ „up-down“

C	-0.4630485438	-0.0948304270	0.1592644346
C	0.0517260416	-0.0431903889	1.6337554535
C	1.5725676021	0.0933559866	1.4995190434
C	1.5260271917	1.3016421629	0.5574460211
C	0.5761116439	0.8530727704	-0.5993697266
C	-0.4039941172	1.3872044599	2.0533217594
H	-0.3227479409	-0.8510012230	2.2612137242
H	2.0515617130	-0.7838519772	1.0595762719
H	2.0644463145	0.3147901773	2.4499611059
H	2.4787329949	1.7044612433	0.2160048068
C	0.6113233191	2.3133615559	1.3120910453
H	1.0607506945	0.3452478181	-1.4297608788
C	-0.0681799704	2.1561250403	-0.9869734055
H	-0.5091775104	-1.0868038766	-0.2836472641
C	-0.5137839064	2.7759889275	0.3133597069
H	1.1257322854	3.0840298071	1.8811747214
C	-1.5511044205	1.8297655160	1.0706498473
H	-0.5677500203	1.5392664221	3.1174943945
C	-1.8069472394	0.5700540683	0.2824157813
H	-2.4061997005	2.3544004014	1.4947962308
H	-0.7886246719	3.8299305037	0.3138773213
N	-2.8761875883	-0.0076592274	-0.1123818782
N	-0.0313416406	2.5873880107	-2.1892821687
N	-0.5226900934	3.8535213502	-2.4668587954
C	-0.3401256805	4.3336263014	-3.7158550717
N	-4.1000699528	0.5902681727	0.1448449364
C	-5.2133359539	-0.1115488021	-0.1582677074
N	-0.7384819219	5.5760517726	-4.0071983852
N	0.2161836265	3.5496658131	-4.6285851757
H	-0.5834497536	5.9733813684	-4.9217024212
H	-1.1644288530	6.1761494059	-3.3181370215
H	0.5268801400	2.6305855158	-4.3408792239
H	0.3564728188	3.8499858019	-5.5810607943
N	-6.4130796807	0.3999093870	0.1353831857
N	-5.0862528638	-1.2869282639	-0.7578421188
H	-7.2602195474	-0.1169436597	-0.0474895540
H	-6.5162697377	1.2936865349	0.5902127740
H	-4.1517215373	-1.6367842111	-0.9259655610
H	-5.8842969577	-1.8425299310	-1.0252635271
H	-4.1734511845	1.4244490637	0.7172224691
H	-0.8236153971	4.4798436287	-1.7279203557

5aH⁺

C	-0.3434733746	-0.0429814848	0.4615979647
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C	0.0983475912	0.0259162579	1.9534364022
C	1.6267933219	-0.0908545582	1.9057220556
C	1.8255339415	1.0573409601	0.9075980569
C	0.8821790785	0.6876977657	-0.2828566303
C	-0.1453375334	1.5308855204	2.2741421637
H	-0.4326566121	-0.6763115501	2.5953474975
H	1.9798838635	-1.0578903445	1.5383428854
H	2.1007358446	0.1073480207	2.8705045152
H	2.8485366631	1.2846938185	0.6069102118
C	1.0455305540	2.2410558457	1.5524895379
H	1.3475159344	0.0366419660	-1.0242542265
C	0.4115829640	2.0375027202	-0.7685495095
H	-0.5223698491	-1.0392638456	0.0671211385
C	0.0729396182	2.8098394983	0.4682199703
H	1.6534094769	2.9475050147	2.1135971874
C	-1.1474651605	2.0824597942	1.2042613702
H	-0.3324844299	1.7631467013	3.3201623180
C	-1.5463217993	0.8695333323	0.4155808762
H	-1.9639275215	2.7332939025	1.5045020785
H	-0.0272944147	3.8833707619	0.3317569110
N	-2.6781150810	0.7491695003	-0.1597849319
N	0.2467904192	2.5210956824	-1.9407949567
N	0.5062259910	1.6855214464	-3.0235815887
C	0.2878261811	2.1747578270	-4.2520725823
N	-2.8028823807	-0.4476059978	-0.8990981802
C	-3.8510093248	-0.6666751218	-1.5120877075
N	0.4902144066	1.3957118272	-5.3247277523
N	-0.1137473225	3.4348205185	-4.3773114954
H	0.2593988015	1.7156685128	-6.2518180872
H	0.8114517405	0.4451721400	-5.2334901650
H	-0.2726403537	3.9595805947	-3.5260758140
H	-0.2353454133	3.8737856243	-5.2753364667
N	-4.7486894604	-0.9292382419	-2.2864402301
H	-5.5685821422	-1.4486585001	-1.9921567626
H	0.6794457821	0.6948980909	-2.8926950543

5bH⁺

C	-0.0786424005	-0.2413585216	0.3686999338
C	0.2316033710	-0.1063868304	1.8882336950
C	1.7488563460	0.1078216233	1.9550972778
C	1.7677746619	1.2893148672	0.9764208426
C	1.0118496260	0.7509782946	-0.2825393053
C	-0.3533977509	1.3055030075	2.1903877378
H	-0.1815102417	-0.9165198729	2.4887055086
H	2.3287418834	-0.7546292756	1.6154706944
H	2.0975814757	0.3876672578	2.9524728449
H	2.7372674204	1.7349637677	0.7522488362
C	0.7089247612	2.2674222219	1.5659813472
H	1.6597971437	0.2325685067	-0.9911567013
C	0.3008468607	1.9808176737	-0.7949517002
H	0.0358442260	-1.2507153751	-0.0238364644

C	-0.2800526826	2.6391536811	0.4140446351
H	1.1107861743	3.0739390216	2.1755414070
C	-1.3662651174	1.6484891589	1.0469106271
H	-0.6630377531	1.4706852125	3.2201174416
C	-1.4524440482	0.3891541378	0.2304000218
H	-2.3211296556	2.1069244231	1.2889945714
H	-0.5946263808	3.6702162886	0.2749498551
N	-2.4803638936	0.0490864576	-0.4382526568
N	0.1218058584	2.4432389053	-1.9737564890
N	0.6276241111	1.7048154878	-3.0407631784
C	0.3759508017	2.1530210256	-4.2777373083
N	-2.4264268319	-1.0781420328	-1.2381022301
N	0.8262946198	1.4680203513	-5.3399348450
N	-0.3123702206	3.2799359680	-4.4233845982
H	0.5711456778	1.7342182634	-6.2774481305
H	1.3999522319	0.6468492185	-5.2337214732
H	-0.6465646099	3.7315670507	-3.5807841337
H	-0.4481473606	3.7143498807	-5.3215610431
H	-3.3694352584	-1.3923756369	-1.4263515956
H	-1.8641343612	-1.8437889022	-0.8722440785
H	0.9986203163	0.7710146948	-2.9043433459

5cH⁺

C	-0.0339207914	-0.3230656055	-0.0259065739
C	0.4611135242	-0.3494139730	1.4372552687
C	1.9569246970	-0.0197928100	1.1929920672
C	1.6529791636	1.3792271332	0.5988464329
C	0.6436118504	1.0139875042	-0.5663630782
C	0.0270885983	0.9052435352	2.2362792880
H	0.2348254829	-1.2788278550	1.9567287896
H	2.4508103447	-0.7083156588	0.5029489412
H	2.5379987376	0.0366406506	2.1145651647
H	2.4994340653	1.9651746321	0.2456947752
C	0.9228519627	1.9977693385	1.8009243019
H	1.1882683670	0.8143090142	-1.4858762687
C	-0.3986361882	2.0636332928	-0.7873611668
H	0.3963468795	-1.1799208233	-0.5507145730
C	-1.0465295960	2.5473710293	0.3273493985
H	1.4401706957	2.6847995825	2.4591664920
C	-0.6183297368	2.2144692981	1.6524126577
H	-0.2551294011	0.7708462129	3.2729047199
C	-1.4791020864	-0.4089875849	-0.1976627515
H	-1.0891289704	2.7858959552	2.4426575923
H	-1.8476320416	3.2677034034	0.1978281002
N	-2.6229144275	-0.4757013187	-0.3294948562
N	-0.8438262963	2.5211492264	-1.9753365860
N	-0.2803896526	2.0510580212	-3.0341494917
C	-0.8458407434	2.5655350523	-4.1880063258
N	-0.2847573984	2.1396131063	-5.3149908963
N	-1.8676833962	3.4083424928	-4.1732021726
H	-0.6054512014	2.4133133256	-6.2307198614

H	0.4857147713	1.4912448094	-5.2418938563
H	-2.2355652149	3.6639641140	-3.2650913684
H	-2.3013079978	3.7698038989	-5.0082121631

Guanidine

C	0.0169736953	0.0121297416	0.1367511141
N	-0.0527707278	0.0525149850	1.4130707999
N	1.1702798691	0.0181841408	-0.6530718260
H	0.8631779346	-0.0397516901	1.8464140107
H	2.0336277065	-0.1141758522	-0.1478448193
H	1.1206580923	-0.5395514734	-1.4950467739
N	-1.1459821420	-0.0319249083	-0.6272680250
H	-1.9733553882	0.1041143237	-0.0634817821
H	-1.1369400398	0.5384607330	-1.4618256984

carbodiimide

C	0.	-0.0840352028	1.0640352028
N	1.2171778240	-0.0057265384	1.0030638042
N	-1.2171778240	-0.0230638042	0.9857265384
H	1.7656767379	0.0236878933	1.8532442214
H	-1.7656767379	-0.8732442214	0.9563121067

ammonia

N	0.1795241369	0.1036476349	-0.0422038709
H	0.0525435249	0.0303373367	0.9616882020
H	1.0643082116	-0.3330725452	-0.2782386516
H	0.2437041301	1.0882525675	-0.2782416795