

Cartesian Coordinates in Ångströms for pyrimidine

RICC2/def2-TZVPP (Turbomole 5.9.1)

S₀

N	-0.000283978	-0.000011097	-0.002025542
N	-0.000284195	-0.000011271	2.400091859
C	0.590341714	-0.000011959	1.199033137
C	-1.340377936	0.000002752	0.015785527
C	-2.068168842	-0.000009165	1.199033015
C	-1.340378148	0.000002604	2.382280583
H	1.670852668	0.000002207	1.199032962
H	-1.834172383	0.000039747	-0.945899586
H	-3.146271500	-0.000043758	1.199033343
H	-1.834172822	0.000039937	3.343965553

S₁

N	-0.420804834	-0.000127812	1.225713868
C	-1.341495775	-0.000323994	0.307975216
N	-0.944772973	0.000080832	-0.983864857
C	0.413280997	-0.000538956	-1.284084394
C	1.377404076	-0.000155642	-0.310224685
C	0.951938546	0.000635468	1.040024465
H	-2.388859188	-0.000865686	0.559722423
H	0.657368654	-0.001150008	-2.334845907
H	2.427770406	-0.000155462	-0.559933205
H	1.584048597	-0.001187685	1.908623061

CASSCF (10,8)/6-311G(2df) (Gaussian 09)

S₀

N	-0.011082483	0.000000090	0.015256017
N	-0.011078604	-0.000000032	2.382805696
C	0.584146282	-0.000000846	1.199034592
C	-1.337113299	0.000000602	0.019913121
C	-2.064796994	0.000000042	1.199035587
C	-1.337116442	0.000000624	2.378150228
H	1.657157249	0.000000144	1.199034899
H	-1.822938305	-0.000000015	-0.938465873
H	-3.137151151	-0.000000651	1.199036497
H	-1.822940961	0.000000042	3.336529147

S₁

N	-0.461453803	-0.000343293	1.272475192
C	-1.328047026	-0.000427418	0.310456311
N	-0.890517789	-0.000432080	-0.935997240
C	0.431500807	-0.000421389	-1.357032366
C	1.363752960	-0.000375929	-0.329708430
C	0.910861914	-0.000303153	0.975521198
H	-2.380589184	-0.000419644	0.504432186
H	0.628233324	-0.000527463	-2.404830085
H	2.414253414	-0.000364718	-0.552374194
H	1.566982556	-0.000173914	1.819363374

Cartesian Coordinates in Ångströms for the σ_A -conformer of pyrimidine-NH₃

Counterpoise corrected MP2/cc-pVTZ (Gaussian 09)

S₀

C	1.983192000	0.736976000	0.000525000
C	2.023438000	-0.651300000	0.000689000
N	0.913308000	-1.398071000	-0.000059000
C	-0.242649000	-0.724834000	-0.001167000
N	-0.399133000	0.605547000	-0.000921000
C	0.727283000	1.328359000	-0.000232000
H	2.886203000	1.328943000	0.001038000
H	2.965192000	-1.185731000	0.001251000
H	0.612361000	2.405035000	-0.000333000
H	-1.153577000	-1.308995000	-0.000997000
N	-3.556890000	-0.096341000	0.000695000
H	-2.743651000	0.510498000	0.000026000
H	-4.106959000	0.168659000	0.807317000
H	-4.108141000	0.168439000	-0.805193000

RICC2/def2-TZVPP (Turbomole 5.9.1)

S₀

C	-0.766046844	-0.000899390	1.909693385
C	0.622680218	-0.000911524	1.954889541
N	1.378257269	0.000168008	0.848301854
C	0.708247888	0.001249901	-0.310767399
N	-0.623003249	0.001405929	-0.475209192
C	-1.350920988	0.000312072	0.650438491
H	-1.361085986	-0.001780734	2.808705089
H	1.151643981	-0.001803547	2.897815246
H	-2.425269260	0.000433751	0.530073411
H	1.293436617	0.002075486	-1.219378801
N	0.078300251	-0.001075484	-3.552018632
H	-0.525261237	0.000487864	-2.736521782
H	-0.175470265	-0.810419415	-4.101429264
H	-0.174432368	0.807046582	-4.103709356

S₁

C	-0.709839029	-1.963200730	0.000238902
C	0.716074573	-1.983693161	0.000275215
N	1.279643961	-0.728758311	-0.000080805
C	0.716768578	0.433960101	-0.000379420
N	-0.656033979	0.469009203	-0.000354205
C	-1.329062496	-0.743403826	-0.000080043
H	-1.273089969	-2.883875151	0.000461760
H	1.355880374	-2.845960098	0.000451854
H	-2.406431693	-0.666569861	-0.000131225
H	1.268176727	1.361018161	-0.000623720
N	0.041325700	3.491538350	0.000275977
H	-0.626284666	2.726779793	-0.000845085
H	-0.168127809	4.060777619	-0.808203178
H	-0.168135948	4.058326994	0.810448297

CASSCF (10,8)/6-311G(2df) (Gaussian 09)**S₀**

C	-0.055536886	0.011663254	0.028793725
C	-0.024241969	-0.005014751	1.414246910
N	1.115790190	-0.017018292	2.090113738
C	2.231876095	-0.012207037	1.374486680
N	2.313712129	0.003273203	0.050177497
C	1.168857662	0.015176182	-0.618713018
H	-0.980111191	0.021297421	-0.514392100
H	-0.928908943	-0.008941946	1.994137728
H	1.235551548	0.027668544	-1.691118188
H	3.160058107	-0.021617527	1.911091614
N	5.664771594	-0.009586213	0.633180423
H	4.867691515	0.001769601	0.026409781
H	6.206344344	-0.816420433	0.394621597
H	6.219729988	0.791867133	0.407638807

S₁

C	-0.095311156	0.003554852	0.033000457
C	-0.083725218	-0.003035325	1.421437418
N	1.190135630	-0.007000655	1.966211426
C	2.346869730	-0.005208413	1.326617174
N	2.342606112	0.000906594	0.030641516
C	1.108437849	0.005447377	-0.643840693
H	-1.028664680	0.007074168	-0.497863031
H	-0.922107592	-0.005285432	2.079430295
H	1.166610997	0.010438731	-1.711567275
H	3.264725535	-0.008870561	1.877475561
N	5.634244046	-0.005180568	0.667545352
H	4.879195061	-0.001375956	0.008443295
H	6.195536745	-0.809089021	0.467780422
H	6.197028654	0.799533345	0.475362707

CASSCF (10,8)/aug-cc-pVDZ (Gaussian 09)**S₀**

C	-0.057829773	0.011722700	0.011886182
C	-0.070996159	0.030341391	1.405377259
N	1.053471589	0.017397941	2.120070012
C	2.195871833	-0.014531826	1.434770727
N	2.321857537	-0.034410439	0.107305307
C	1.192602914	-0.021189209	-0.600820980
H	-0.970249624	0.022274522	-0.563799771
H	-0.998768515	0.056149357	1.959414964
H	1.292255943	-0.037306986	-1.676986854
H	3.110880337	-0.025334785	2.005890882
N	5.732046903	-0.023724610	0.591659720
H	4.878650680	-0.064127927	0.062863450
H	6.322718464	-0.773103820	0.280729110
H	6.193072102	0.837752827	0.362315186

S₁

C	-0.115583873	0.003365997	0.028010430
C	-0.109767681	-0.003117351	1.424531226
N	1.166328618	-0.006630715	1.976476766
C	2.331394153	-0.004440254	1.337871403
N	2.333085678	0.001693553	0.033386429
C	1.097924573	0.005721900	-0.648596636
H	-1.052361603	0.006496454	-0.509980175
H	-0.958330161	-0.005863177	2.080806362
H	1.157921171	0.010747446	-1.722990206
H	3.252471283	-0.007763275	1.895446791
N	5.681208580	-0.005903532	0.659082210
H	4.920824985	-0.000986812	0.001861762
H	6.243987208	-0.814567418	0.467757037
H	6.246478839	0.803156320	0.477011227

Cartesian Coordinates in Ångströms for the σ_B -complex**Counterpoise corrected MP2/cc-pVTZ (Gaussian 03)****S₀**

C	0.951590000	1.346447000	-0.000068000
C	2.076193000	0.531991000	0.000303000
N	1.989978000	-0.803899000	0.000289000
C	0.750222000	-1.302651000	-0.000107000
N	-0.398880000	-0.618397000	-0.000466000
C	-0.286742000	0.717471000	-0.000409000
H	1.034979000	2.422983000	-0.000059000
H	3.074640000	0.950900000	0.000540000
H	-1.217169000	1.271532000	-0.000613000
H	0.667131000	-2.381691000	-0.000104000
N	-3.529704000	0.105493000	0.000284000
H	-2.750100000	-0.544422000	0.000337000
H	-4.093521000	-0.130840000	-0.805757000
H	-4.093304000	-0.130393000	0.806599000

RICC2/def2-TZVPP (Turbomole 5.9.1)**S₀**

N	-0.765920773	0.000109603	1.911932890
C	0.573049446	0.000101692	1.981830007
C	1.377638851	-0.000022077	0.849614425
C	0.735518900	-0.000148746	-0.382209645
N	-0.603790791	-0.000170162	-0.482596660
C	-1.275618880	-0.000027623	0.675463764
H	1.001678805	0.000182651	2.974287629
H	-2.353902744	-0.000034296	0.602844072
H	1.276856060	-0.000250862	-1.318411264
N	0.056490375	0.000088092	-3.549209023
H	-0.566083960	-0.000091595	-2.747562012
H	-0.186425827	-0.807928990	-4.105619316
H	-0.185773457	0.808939513	-4.104698759
H	2.453284671	-0.000046081	0.922340070

S₁

N	-0.787483312	-1.768612169	0.000530871
C	0.550421736	-2.063943134	0.000690703
C	1.396014050	-0.906872203	-0.000119642
C	0.791317968	0.318209245	-0.000892727
N	-0.581539629	0.498308488	-0.000925557
C	-1.378428378	-0.618036597	-0.000190562
H	0.858176339	-3.092916854	0.001256277
H	-2.451190425	-0.528020002	-0.000205702
H	1.359590113	1.238093101	-0.001495280
N	0.101078199	3.536385302	0.000596325
H	-0.490546670	2.711563158	-0.001298405
H	-0.163187453	4.084384443	-0.806576112
H	-0.161689299	4.079106334	0.811749835
H	2.470180041	-1.008004870	-0.000128775

CASSCF (10,8)/6-311G(2df) (Gaussian 09)**S₀**

C	-0.024494598	-0.000398277	0.015574318
C	-0.043202924	0.000377249	1.400580754
N	1.073098900	0.000678789	2.117201120
C	2.209480091	-0.000018848	1.437365505
N	2.341178354	-0.000741766	0.118802068
C	1.220656568	-0.001100496	-0.593581904
H	-0.929856249	-0.000269963	-0.559129602
H	-0.967285850	0.001280285	1.948901789
H	1.333695274	-0.001424436	-1.661192135
H	3.115278959	0.000385343	2.012861311
N	3.734395311	-0.001759842	-2.962415273
H	3.823391234	-0.001918281	-1.964238812
H	4.224355578	0.802381694	-3.301227076
H	4.225193710	-0.805223122	-3.301617122

S₁

C	-0.092689135	-0.009095966	0.026520411
C	-0.129567656	-0.001274112	1.414954626
N	1.123953495	0.010044096	2.008914225
C	2.299864248	0.014201707	1.404584541
N	2.339955315	0.007016317	0.112223802
C	1.131478057	-0.005104535	-0.611962362
H	-1.007483869	-0.018162163	-0.535538526
H	-0.990838397	-0.003193392	2.042740817
H	1.237270083	-0.010510649	-1.675429162
H	3.193283363	0.023449916	1.994610564
N	3.801295433	-0.005261188	-2.978211542
H	3.776884143	0.003376624	-1.976689495
H	4.324535805	0.797475247	-3.266470032
H	4.327942051	-0.810712902	-3.252362267

CASSCF (10,8)/aug-cc-pVDZ (Gaussian 09)

S₀

C	-0.054102070	0.000224800	0.034503354
C	-0.056422286	0.001268302	1.427573831
N	1.074838750	0.000732359	2.133226428
C	2.208349012	-0.000819967	1.435001173
N	2.325764162	-0.001894168	0.108015068
C	1.190369024	-0.001436295	-0.593266329
H	-0.971887856	0.000662532	-0.532593834
H	-0.979371677	0.002540888	1.990127702
H	1.288080788	-0.002303514	-1.668880509
H	3.126165945	-0.001274058	2.002897871
N	3.786689347	-0.001220043	-2.994374599
H	3.831821070	-0.003373778	-1.990430974
H	4.282675361	0.808217492	-3.320186963
H	4.282914803	-0.809076215	-3.323727275

S₁

C	-0.140145177	-0.015929629	0.057778920
C	-0.142882095	-0.009859605	1.454720810
N	1.129497458	0.011998800	2.018095588
C	2.296072042	0.026332901	1.381902517
N	2.305551380	0.020636514	0.080143866
C	1.075357286	-0.000481807	-0.614719445
H	-1.073919543	-0.032434257	-0.484942598
H	-0.995638146	-0.020392793	2.105458529
H	1.149666191	-0.004081633	-1.687733449
H	3.209500794	0.042401464	1.952023813
N	3.888065886	-0.004459983	-3.014506941
H	3.779359454	0.013850829	-2.015790640
H	4.441244075	0.791148018	-3.275853900
H	4.414153333	-0.826479817	-3.248691475

Cartesian Coordinates in Ångströms for the π -complex

Counterpoise corrected MP2/cc-pVTZ (Gaussian 03)

S₀

C	-0.951382000	0.011646000	-1.239187000
C	-0.776873000	1.188736000	-0.524718000
N	-0.468825000	1.193259000	0.778048000
C	-0.340379000	-0.010479000	1.345990000
N	-0.475940000	-1.204378000	0.759228000
C	-0.784168000	-1.177539000	-0.543230000
H	-1.194330000	0.020604000	-2.290935000
H	-0.880084000	2.155752000	-1.000345000
H	-0.893626000	-2.136334000	-1.033893000
H	-0.095804000	-0.019479000	2.400423000
N	2.637112000	0.000160000	-0.417488000
H	2.346118000	0.799516000	0.131478000
H	3.648508000	-0.004486000	-0.385501000
H	2.339603000	-0.813039000	0.107126000

RICC2/def2-TZVPP (Turbomole 5.9.1)

S₀			
C	-0.053075489	-0.957094362	1.232720000
C	1.154772942	-0.764742174	0.576488563
N	1.221333365	-0.380485718	-0.706424840
C	0.042137839	-0.193265893	-1.310761272
N	-1.179164844	-0.330503567	-0.781161448
C	-1.208723738	-0.715657915	0.502848792
H	-0.091582817	-1.264728852	2.265023668
H	2.097917922	-0.917159705	1.082089341
H	-2.187023370	-0.828294694	0.948499423
H	0.080688074	0.107566521	-2.348460511
N	0.015058061	2.577657067	0.461381092
H	0.839410676	2.363355675	-0.084204917
H	0.014900007	3.579317722	0.598854367
H	-0.776305914	2.369431202	-0.133328499

CASSCF (10,8)/6-311G(2df) (Gaussian 09)

S₀			
C	-0.013764190	-0.062382942	-0.004709629
C	-0.010905504	-0.105268476	1.379397709
N	1.116090959	-0.153234828	2.076732433
C	2.241696434	-0.156414058	1.378351981
N	2.354930782	-0.111852916	0.059130345
C	1.222264431	-0.064253459	-0.629085400
H	-0.926967571	-0.017607866	-0.564502445
H	-0.926152194	-0.099260401	1.941951485
H	1.309264695	-0.024647680	-1.699145654
H	3.156127151	-0.199362704	1.938915516
N	1.443388876	3.497903633	0.897160409
H	1.464464148	3.224253980	1.859625640
H	1.459252223	4.498297738	0.878100788
H	2.302280138	3.184360101	0.490134979

CASSCF (10,8)/aug-cc-pVDZ (Gaussian 09)

S₀			
C	-0.054168000	-0.213316000	-0.038003000
C	-0.053316000	-0.224491000	1.355009000
N	1.078852000	-0.253914000	2.056165000
C	2.209566000	-0.270744000	1.352753000
N	2.325923000	-0.259615000	0.028310000
C	1.188725000	-0.230723000	-0.665484000
H	-0.972671000	-0.191647000	-0.603344000
H	-0.975834000	-0.212432000	1.917894000
H	1.275794000	-0.224100000	-1.742704000
H	3.128582000	-0.298984000	1.918170000
N	1.558042000	3.807130000	0.992608000
H	1.643703000	3.588177000	1.968368000
H	1.400300000	4.794470000	0.905404000
H	2.438470000	3.600718000	0.556912000