Electronic Supplementary Information

Functionalization of pyrimidine and purine to RNA bases in water/ammonia ices via radical substitution reactions

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Contents

I. Optimized coordinates (Å) and vibrational frequencies (cm^{-1}) in adenine pathways

1) ωB97X-D/6-311G(d,p) without SCRF

Reactants

Purine

Cartesian coordinates

N	2.101040	0.676994	0.000006
C	2.010720	-0.663575	-0.000005
N	0.915707	-1.409624	-0.000001
C	-0.216129	-0.710117	0.000002
C	-0.234369	0.697105	-0.000003
C	0.973162	1.374888	0.000003
N	-1.501201	-1.209348	0.000004
C	-2.255799	-0.149108	0.000000
N	-1.568244	1.034548	0.000000
H	2.956709	-1.195150	-0.000019
H	1.050520	2.458811	0.000008
H	-3.336764	-0.163908	0.000002
H	-1.967083	1.957106	-0.000033

Vibrational frequencies

224.2068	250.9018	431.6364
461.0837	466.0263	577.2683
632.9234	659.3659	667.9578
814.1524	836.4483	910.4047
919.1085	934.1613	954.0796
1000.2169	1119.3938	1154.7424
1212.9088	1269.0375	1311.5945
1334.5058	1388.9827	1438.8965
1448.5542	1523.7336	1559.5394
1637.5388	1690.2884	3176.4602
3203.1098	3259.6241	3705.0181

Amino radical

Cartesian coordinates

N	0.000000	0.000000	0.143154
H	0.000000	0.801075	-0.501039
H	0.000000	-0.801075	-0.501039

Vibrational frequencies

1529.3682	3392.4285	3483.9661

Intermediate

i1

Cartesian coordinates

N	-1.985583	0.501067	0.158974
C	-1.380650	1.626307	-0.035649
N	-0.032633	1.914422	-0.115159
C	0.737295	0.830505	-0.022441
C	0.230405	-0.453526	0.177720
C	-1.212112	-0.713584	0.380007

N	2.117085	0.780186	-0.152133
C	2.408333	-0.478759	-0.042746
N	1.300962	-1.279698	0.163347
N	-1.647055	-1.851866	-0.415536
H	-2.018818	2.495535	-0.178365
H	-1.378284	-0.988186	1.434254
H	3.400180	-0.902066	-0.104620
H	1.269728	-2.284033	0.225291
H	-1.623361	-1.588260	-1.396202
H	-2.618511	-2.047421	-0.198152

Vibrational frequencies

99.3447	169.7576	262.6257
297.6921	326.1874	434.1065
485.5790	517.8179	571.4544
588.0025	641.9897	679.4934
731.5243	801.8642	874.9059
890.5092	907.5197	953.2621
985.0685	1023.8859	1070.4980
1100.6371	1175.2789	1198.7360
1227.0510	1266.1839	1319.4063
1381.8043	1389.4872	1415.4439
1417.9645	1441.1326	1531.0709
1580.2485	1611.1875	1678.4951
2976.7737	3172.5162	3263.3119
3524.8819	3606.1865	3690.3441

Transition states

ts1a

Cartesian coordinates

N	-1.951122	0.298737	0.540257
C	-1.512837	1.456754	0.044132
N	-0.271730	1.800497	-0.299548
C	0.626235	0.829845	-0.116204
C	0.286501	-0.429123	0.393350
C	-1.066805	-0.724346	0.663629
N	1.979104	0.888394	-0.384890
C	2.421425	-0.291573	-0.063635
N	1.452880	-1.139707	0.413046
N	-1.518789	-1.861122	-0.940837
H	-2.268616	2.226713	-0.078289
H	-1.357505	-1.546284	1.306793
H	3.450783	-0.610381	-0.145810
H	1.568187	-2.104817	0.670183
H	-1.221006	-1.216101	-1.681067
H	-2.531349	-1.706076	-0.895638

Vibrational frequencies

-582.0776	113.4229	117.5749
213.9651	251.6185	267.4035
451.3198	461.4840	504.4154
566.1923	615.8280	656.9134

668.5612	741.8658	807.8422
824.8286	843.2245	903.3425
925.1219	958.3480	976.6646
1000.5854	1106.5244	1127.3083
1205.7281	1266.1048	1286.2330
1328.2210	1382.1006	1423.9834
1443.1234	1492.8957	1539.2929
1562.2507	1596.8909	1643.4599
3185.4644	3198.7709	3261.3002
3419.1021	3514.2326	3703.3886

ts1b

Cartesian coordinates

N	-1.932187	0.530939	-0.012789
C	-1.285340	1.700418	-0.021022
N	0.022559	1.926764	-0.040117
C	0.760228	0.811105	-0.036137
C	0.200781	-0.469268	-0.000120
C	-1.202843	-0.600347	0.089436
N	2.136679	0.725551	-0.048483
C	2.384568	-0.551012	-0.001037
N	1.261230	-1.336948	0.027345
N	-1.832679	-1.835461	-0.077743
H	-1.922187	2.579672	-0.042482
H	-1.114904	-0.595355	1.794476
H	3.371640	-0.990853	0.006295
H	1.227157	-2.335626	0.135717
H	-1.462741	-2.365806	-0.854102
H	-2.832536	-1.713313	-0.164103

Vibrational frequencies

-1235.3553	160.1994	190.6286
215.3654	293.1024	301.4695
469.6753	481.5445	501.2048
549.2877	587.1185	610.7414
646.0844	648.6750	687.7766
735.6163	774.0727	843.8496
891.2663	904.1014	957.0707
1002.1946	1061.1903	1104.8879
1143.9161	1255.7043	1299.6691
1306.8736	1355.2062	1395.4653
1423.4750	1435.9708	1496.2050
1556.1971	1611.2265	1656.7394
1669.0437	3186.5610	3264.4919
3576.0909	3674.9397	3706.4994

Product

Adenine

N	-1.940879	-0.493164	-0.015177
C	-1.308012	-1.680596	-0.010925
N	-0.011794	-1.921298	0.016224
C	0.733095	-0.807624	0.015750

C	0.183182	0.476652	-0.007857
C	-1.208570	0.612114	-0.006737
N	2.109983	-0.737505	0.021795
C	2.371614	0.537534	-0.006340
N	1.262530	1.336545	-0.015403
N	-1.852293	1.825553	-0.047537
H	-1.962285	-2.547149	-0.022553
H	3.364646	0.964288	-0.020630
H	1.254292	2.335198	-0.122652
H	-1.412254	2.596626	0.427383
H	-2.845081	1.751638	0.115799

Vibrational frequencies

159.8535	208.4082	289.0789
307.1287	367.9395	423.9043
530.9625	541.9434	565.2959
596.7267	622.2876	647.8969
719.8989	736.2643	830.5971
895.7232	906.9398	957.5899
1002.9256	1053.3574	1114.1324
1151.7063	1252.4326	1303.7131
1334.0260	1366.6057	1407.8133
1429.0476	1450.9437	1537.7337
1564.6307	1628.9780	1669.2541
1704.9950	3187.9904	3260.0500
3607.6093	3711.0828	3721.3306

2) SCRF/PCM//ωB97X-D/6-311G(d,p)

Reactants

Purine

Cartesian coordinates

N	-2.097381	0.683103	0.000000
C	-2.015751	-0.657382	0.000000
N	-0.922722	-1.409172	-0.000001
C	0.214254	-0.711655	0.000000
C	0.239015	0.694984	0.000001
C	-0.963353	1.379158	0.000000
N	1.493494	-1.214995	-0.000001
C	2.254796	-0.147891	0.000000
N	1.570850	1.025597	0.000001
H	-2.964463	-1.185107	0.000000
H	-1.028405	2.462354	0.000001
H	3.334966	-0.160862	0.000000
H	1.974446	1.948595	0.000002

Vibrational frequencies

226.5121	253.0693	431.7686
460.9601	541.6683	578.2088
637.7338	662.8836	667.6017
815.6401	838.9376	923.4836
937.5805	947.3466	957.5907

1002.0850	1135.5150	1150.6831
1220.7233	1277.8281	1311.9522
1333.0806	1385.5013	1448.0254
1450.5620	1521.2227	1546.1581
1636.2018	1690.1832	3194.6077
3200.4407	3273.7007	3679.9414

Amino radical

Cartesian coordinates

N	0.000000	0.000000	0.142999
H	0.000000	0.799869	-0.500496
H	0.000000	-0.799869	-0.500496

Vibrational frequencies

1532.8411	3414.1577	3497.4449

Intermediate

i1

Cartesian coordinates

N	1.982831	0.499680	-0.184766
C	1.384417	1.623810	0.023261
N	0.035710	1.910933	0.127962
C	-0.733584	0.829093	0.033650
C	-0.233656	-0.460231	-0.178990
C	1.209731	-0.725984	-0.379427
N	-2.112897	0.785650	0.163282
C	-2.410516	-0.476116	0.037419
N	-1.308816	-1.273522	-0.172097
N	1.654428	-1.840915	0.438995
H	2.024049	2.494827	0.152450
H	1.368150	-1.020054	-1.428073
H	-3.401578	-0.900735	0.089799
H	-1.304724	-2.276810	-0.274074
H	1.635498	-1.563933	1.415809
H	2.621468	-2.049517	0.214979

Vibrational frequencies

89.8239	173.7202	262.6687
297.7151	316.3014	437.8509
484.5162	519.8947	588.6920
592.2834	646.0808	676.3096
733.8204	805.9766	881.4071
897.8795	904.5021	953.8601
983.2554	1007.8911	1081.3144
1109.1265	1174.7839	1198.2013
1225.7601	1271.1269	1318.8582
1388.2176	1396.7015	1416.5496
1428.9454	1447.4253	1523.1459
1595.2897	1613.1718	1665.4636
2996.3379	3161.9404	3277.1544
3529.1462	3611.1240	3673.2885

Transition states

ts1a

Cartesian coordinates

N	1.943469	0.291333	-0.560333
C	1.516599	1.449879	-0.060283
N	0.278839	1.795047	0.301300
C	-0.622893	0.824024	0.126147
C	-0.293087	-0.437286	-0.385178
C	1.056970	-0.737183	-0.665384
N	-1.973015	0.893243	0.393737
C	-2.425789	-0.288578	0.061804
N	-1.464578	-1.134958	-0.408288
N	1.543167	-1.840798	0.953763
H	2.274580	2.219910	0.049615
H	1.336095	-1.564066	-1.305712
H	-3.456406	-0.602798	0.134630
H	-1.604245	-2.084884	-0.713893
H	1.214393	-1.210212	1.692763
H	2.549615	-1.650158	0.918697

Vibrational frequencies

-583.2342	116.5239	124.2351
168.1708	252.7033	271.5953
452.4978	464.9391	552.0726
567.0188	618.6021	657.6100
669.6360	744.5626	810.8053
816.6151	842.9774	924.7508
928.9376	960.7851	976.1568
999.6714	1118.3019	1127.8922
1212.7062	1271.3269	1288.8827
1329.7688	1379.7761	1430.2875
1443.0666	1496.8169	1523.9891
1548.1525	1604.0832	1641.8539
3181.1093	3212.9759	3273.8837
3424.2779	3517.6740	3678.4924

ts1b

Cartesian coordinates

N	-1.938416	0.522929	-0.027290
C	-1.298666	1.690868	-0.035220
N	0.010095	1.929025	-0.025554
C	0.754204	0.811766	-0.020261
C	0.208966	-0.474718	-0.000895
C	-1.203339	-0.618058	0.095109
N	2.128166	0.742103	-0.035835
C	2.390178	-0.541170	-0.014603
N	1.278373	-1.326889	0.012032
N	-1.851613	-1.814079	-0.066187
H	-1.940750	2.566603	-0.076528
H	-1.038427	-0.524080	1.742480
H	3.377913	-0.977125	-0.025176
H	1.269796	-2.333780	0.037266

H	-1.345890	-2.579449	-0.479482
H	-2.816933	-1.735913	-0.343502

Vibrational frequencies

-1233.1568	162.3074	202.4269
253.1640	301.2754	313.5232
398.7430	494.0876	506.2611
539.5897	556.9904	596.4461
613.9460	658.4078	674.7817
723.8167	764.6853	844.3801
908.9725	909.5812	961.0857
1003.5177	1035.2686	1129.0408
1160.4944	1265.9927	1294.3422
1327.8408	1362.1576	1395.9875
1421.8176	1450.4473	1497.4997
1541.0863	1608.7617	1642.4128
1663.8843	3176.3730	3278.9117
3622.4458	3689.4660	3738.2949

Product

Adenine

Cartesian coordinates

N	1.945450	0.486712	-0.002249
C	1.320018	1.674779	-0.000778
N	0.023641	1.927215	0.004465
C	-0.727393	0.809772	0.003658
C	-0.188291	-0.476335	-0.002783
C	1.207706	-0.626749	-0.003172
N	-2.101399	0.751948	0.005952
C	-2.372733	-0.531740	-0.000445
N	-1.273393	-1.324642	-0.005682
N	1.840365	-1.822058	-0.041210
H	1.980592	2.537766	-0.001083
H	-3.365442	-0.957041	-0.002309
H	-1.278274	-2.331330	-0.019400
H	1.350323	-2.667393	0.195338
H	2.834306	-1.814594	0.119641

Vibrational frequencies

145.6328	208.2269	264.6815
290.1103	309.3806	463.6040
502.6306	528.8627	545.7772
588.4454	622.2306	650.0201
716.0660	736.8633	830.7575
911.5760	916.3840	963.1477
1005.1462	1030.2080	1131.5242
1170.8357	1254.8694	1301.5157
1350.6280	1371.3838	1403.6564
1434.3597	1472.3744	1537.4103
1550.9193	1621.4968	1647.4422
1693.7005	3175.8585	3274.9005
3626.9722	3688.3041	3748.8974

3) SCRF/SMD//ωB97X-D/6-311G(d,p)

Reactants

Purine

Cartesian coordinates

N	-2.097644	0.686033	0.000000
C	-2.015456	-0.654410	-0.000001
N	-0.924176	-1.409160	-0.000001
C	0.213494	-0.711042	0.000000
C	0.239179	0.692141	0.000000
C	-0.958678	1.378786	0.000001
N	1.490511	-1.217560	0.000000
C	2.252989	-0.146749	0.000000
N	1.571416	1.023485	0.000001
H	-2.962317	-1.182562	-0.000001
H	-1.016601	2.461534	0.000001
H	3.332675	-0.158928	0.000000
H	1.976331	1.948014	0.000001

Vibrational frequencies

221.1206	258.4265	433.4567
466.2991	502.4767	581.0672
632.8638	661.1738	668.4868
816.7300	845.2022	927.2968
951.7517	959.8514	962.0066
1003.0036	1122.9158	1147.7994
1226.2797	1285.0949	1309.0466
1330.1914	1393.4417	1436.4152
1454.3231	1528.7404	1545.0939
1642.2836	1695.7728	3216.9941
3222.0152	3293.0884	3670.8111

Amino radical

Cartesian coordinates

N	0.000000	0.000000	0.143121
H	0.000000	0.799395	-0.500923
H	0.000000	-0.799395	-0.500923

Vibrational frequencies

1497.6472	3413.7451	3493.0780

Intermediate

i1

Cartesian coordinates

N	1.982139	0.494998	-0.205905
C	1.385664	1.618344	0.014062
N	0.039750	1.908150	0.138091
C	-0.730279	0.826613	0.043156
C	-0.234378	-0.462115	-0.174472
C	1.204015	-0.732317	-0.376319
N	-2.109708	0.789856	0.169485

C	-2.409716	-0.472182	0.032020
N	-1.313685	-1.270474	-0.179149
N	1.658031	-1.835991	0.452297
H	2.026933	2.487843	0.131813
H	1.350144	-1.040936	-1.419554
H	-3.402045	-0.893531	0.075725
H	-1.322495	-2.273279	-0.303407
H	1.625846	-1.542412	1.424756
H	2.634089	-2.013513	0.236243

Vibrational frequencies

100.8657	186.8015	263.6021
315.2149	400.2235	446.1979
487.8285	526.7385	575.3180
601.2276	640.1219	678.4966
740.4007	812.8922	897.6731
902.8780	920.7165	955.0264
992.5583	1022.6249	1082.0354
1112.8722	1184.7922	1203.6911
1232.2699	1280.7879	1337.7629
1389.5330	1408.8279	1416.0271
1443.3946	1460.8202	1528.3063
1604.8540	1611.0272	1632.7998
3036.7162	3190.6741	3295.2212
3517.3687	3599.0793	3641.8862

Transition states

ts1a

Cartesian coordinates

N	1.946356	0.258688	-0.585317
C	1.540153	1.420154	-0.070487
N	0.314082	1.779595	0.311615
C	-0.604424	0.824718	0.131103
C	-0.297781	-0.432240	-0.397830
C	1.040957	-0.750854	-0.681768
N	-1.950601	0.914129	0.408513
C	-2.422201	-0.259447	0.060139
N	-1.480963	-1.111707	-0.425469
N	1.496967	-1.835543	0.998289
H	2.309024	2.178235	0.034790
H	1.308439	-1.601654	-1.293585
H	-3.456967	-0.558191	0.130958
H	-1.638400	-2.057427	-0.741380
H	1.152564	-1.164005	1.693517
H	2.504227	-1.647081	0.975337

Vibrational frequencies

-683.3519	112.6075	118.9258
134.9714	250.8326	275.2410
453.4509	464.2411	521.7394
569.9061	620.4517	659.2363
666.6019	729.1113	799.9312

815.2536	835.9247	927.0339
936.9758	961.2039	966.9388
995.6726	1112.6965	1121.9375
1218.0107	1275.5057	1288.3561
1331.0241	1382.7012	1425.8646
1447.6035	1503.3511	1518.8832
1524.3521	1616.8384	1648.1817
3203.9675	3226.6589	3293.7546
3422.7953	3514.0405	3659.2679

ts1b

Cartesian coordinates

N	-1.937974	0.521567	-0.048141
C	-1.296721	1.692412	-0.033575
N	0.008710	1.934822	-0.001362
C	0.752546	0.815054	-0.007579
C	0.204071	-0.465776	-0.022779
C	-1.201005	-0.612199	0.043300
N	2.125324	0.743103	-0.006026
C	2.379763	-0.546199	-0.013117
N	1.269960	-1.324383	-0.017563
N	-1.828906	-1.808611	-0.166449
H	-1.940241	2.565928	-0.062396
H	-1.026701	-0.575301	1.769540
H	3.365996	-0.984030	-0.023830
H	1.249198	-2.333555	-0.032351
H	-1.331146	-2.629133	0.148697
H	-2.808821	-1.809153	0.079619

Vibrational frequencies

-1240.0983	149.4060	196.7765
298.2579	303.4743	395.1232
432.6610	468.2574	524.4623
548.0873	557.1511	578.4610
623.7520	629.1414	655.4236
717.9822	746.8862	825.6354
909.0430	911.7996	957.9702
1010.5057	1044.6682	1100.9370
1160.5334	1252.9621	1298.8507
1336.3342	1375.1864	1397.1576
1428.3684	1436.8100	1515.0363
1537.7045	1617.7534	1632.8034
1671.9602	3202.7031	3297.1100
3586.2892	3652.2789	3693.1264

Product

Adenine

Cartesian coordinates

N	1.952516	0.476855	0.000811
C	1.331068	1.666940	0.001739
N	0.036329	1.931297	0.001659
C	-0.721464	0.815444	0.000742

C	-0.188823	-0.468548	-0.001633
C	1.203815	-0.632708	-0.003619
N	-2.095103	0.763213	0.002310
C	-2.368076	-0.523909	0.000871
N	-1.273606	-1.315976	-0.001642
N	1.810513	-1.835881	-0.042127
H	1.996076	2.524925	0.004336
H	-3.361541	-0.945657	0.001246
H	-1.270764	-2.325152	-0.003164
H	1.279568	-2.669559	0.151667
H	2.803005	-1.864417	0.130247

Vibrational frequencies

153.4019	206.3127	243.7188
312.5022	324.9996	476.6264
519.4301	531.2596	547.3778
584.9976	624.3271	655.6779
722.6873	740.9857	830.2630
912.5744	913.0117	961.5487
1012.3886	1039.8194	1110.4122
1167.0300	1248.4649	1298.5781
1358.1544	1383.1126	1404.8591
1443.9908	1451.8140	1540.4484
1551.8300	1627.6129	1638.4008
1697.8666	3202.4809	3294.4106
3609.4682	3654.0798	3732.9117

II. Optimized coordinates (Å) and vibrational frequencies (cm^{-1}) in guanine pathways

1) ωB97X-D/6-311G(d,p) without SCRF/PCM

Reactants

purine

Cartesian coordinates

C	0.973208	1.374751	-0.000041
N	2.101088	0.677065	-0.000087
C	2.010766	-0.663564	-0.000037
N	0.915790	-1.409574	0.000074
C	-0.216140	-0.710159	0.000089
C	-0.234493	0.696884	0.000082
N	-1.501319	-1.209174	-0.000092
N	-1.568166	1.034630	0.000223
C	-2.255918	-0.149150	-0.000123
H	-3.336962	-0.164054	-0.000146
H	-1.966358	1.957277	-0.000496
H	1.050199	2.458871	-0.000050
H	2.956841	-1.195297	0.000046

Vibrational frequencies

224.3273	250.8820	431.8278
461.0177	463.8186	577.2538
632.8685	659.3466	667.9730
814.1358	836.4406	910.6309
919.1577	934.7253	954.1823
1000.7124	1118.7104	1154.7999
1213.0025	1269.1049	1311.7558
1334.6682	1389.1413	1438.4315
1448.8734	1523.8124	1559.8939
1637.6603	1690.1372	3174.9081
3201.7181	3258.9131	3706.9715

amino radical

Cartesian coordinates

N	0.000000	0.000000	0.143114
H	0.000000	0.800998	-0.500899
H	0.000000	-0.800998	-0.500899

Vibrational frequencies

1528.9608	3394.2251	3485.8469

hydroxyl radical

Cartesian coordinates

O	0.000000	0.000000	0.107778
H	0.000000	0.000000	-0.862222

Vibrational frequencies

3793.3874

Intermediates

i2-complex

Cartesian coordinates

C	0.968135	0.928093	-0.912749
N	2.102947	0.341090	-0.554415
C	2.025976	-0.818128	0.120813
N	0.938786	-1.475676	0.501108
C	-0.201399	-0.890489	0.142823
C	-0.234804	0.323327	-0.575920
N	-1.478250	-1.333542	0.396743
N	-1.568923	0.583125	-0.770043
C	-2.242211	-0.428293	-0.145350
H	-3.322860	-0.449778	-0.129636
H	-1.971858	1.425103	-1.142509
H	2.977256	-1.267847	0.387113
O	-0.144864	1.934495	1.458793
H	0.589564	1.454580	1.872034
H	1.030709	1.869942	-1.448814

Vibrational frequencies

23.5610	70.3725	112.8648
136.2937	223.7166	251.6160
427.9201	431.9824	463.6084
492.6871	576.7383	626.9730
655.1872	668.7222	813.7382
829.1523	916.3739	920.9409
941.3044	954.7365	1000.6695
1126.1960	1153.4967	1215.1382
1266.9788	1310.2751	1336.1104
1389.8081	1442.2794	1448.7977
1520.7911	1555.8681	1632.7140
1684.4885	3190.9012	3201.7893
3261.0633	3709.7448	3798.6753

i3

Cartesian coordinates

C	1.195000	-0.743605	0.368241
N	1.992019	0.435939	0.128456
C	1.418732	1.580991	-0.038532
N	0.077682	1.900267	-0.090938
C	-0.716217	0.834805	-0.015610
C	-0.241678	-0.468771	0.150573
N	-2.097616	0.823117	-0.133784
N	-1.333695	-1.264128	0.134576
C	-2.421188	-0.428525	-0.049118
H	-3.423664	-0.825271	-0.115667
H	-1.339938	-2.270042	0.169072
H	2.078261	2.432995	-0.183468
O	1.611668	-1.815115	-0.443187
H	2.565885	-1.730455	-0.519449
H	1.349478	-1.002028	1.433524

Vibrational frequencies

96.1930	168.8148	231.4557
265.1699	338.0938	442.1369
478.3234	519.4105	563.4912
592.2518	641.0178	684.1076
733.1112	830.0032	877.7245
902.0015	950.6728	979.9342
1000.2540	1075.1460	1106.0605
1172.5149	1219.2487	1258.4895
1279.2815	1326.1839	1383.3160
1387.4204	1421.2474	1426.7789
1453.7292	1534.7289	1587.9963
1618.1742	2914.2190	3181.3005
3264.1807	3691.8788	3882.0916

7H-purin-6-ol

Cartesian coordinates

C	1.177201	-0.657767	0.000158
N	1.958436	0.399595	0.000052
C	1.376384	1.617782	-0.000048
N	0.090963	1.902573	-0.000081
C	-0.701262	0.820815	-0.000127
C	-0.202084	-0.486022	0.000053
N	-2.077093	0.800197	0.000176
N	-1.305273	-1.304747	-0.000213
C	-2.383752	-0.467469	0.000062
H	-3.391822	-0.857255	0.000147
H	-1.313292	-2.309678	-0.000196
H	2.065267	2.456210	-0.000097
O	1.712802	-1.883981	0.000000
H	2.669275	-1.764781	0.000030

Vibrational frequencies

171.1503	217.0268	296.0354
312.1905	482.6776	534.6979
535.8147	553.3024	592.9280
626.2536	649.3969	716.9187
737.5602	828.5770	902.9620
902.9804	960.3857	998.3751
1094.1709	1128.6511	1174.2069
1272.3464	1305.4376	1353.0998
1375.1597	1415.2460	1436.6002
1455.1496	1546.9542	1561.2420
1641.7993	1730.9519	3202.6098
3261.5328	3710.3751	3844.1154

1H-purin-6(7H)-one

Cartesian coordinates

C	1.124571	0.908382	0.000228
N	1.931090	-0.243093	-0.000548
C	1.470867	-1.536097	-0.000064
N	0.233445	-1.887966	0.000265
C	-0.640279	-0.832787	-0.000038

C	-0.245863	0.494473	-0.000707
N	-2.003241	-0.925943	0.000668
N	-1.404002	1.224042	-0.000294
C	-2.417460	0.317714	-0.000210
H	-3.453162	0.623737	-0.000186
H	-1.469892	2.228056	-0.000487
H	2.244651	-2.297285	-0.000072
O	1.587513	2.029719	0.000670
H	2.926236	-0.071653	-0.000502

Vibrational frequencies

161.6726	193.2436	281.7366
307.0085	519.9928	545.4320
555.9314	570.2779	618.9483
644.0789	682.7146	721.4534
759.4673	814.9792	884.0174
913.3343	958.2287	970.1938
1098.3004	1120.9258	1142.4467
1222.5118	1312.6907	1371.7535
1431.0932	1440.0624	1462.7375
1500.7475	1579.3488	1591.0063
1684.5686	1838.0574	3202.2482
3262.5422	3643.5818	3698.9640

i4

Cartesian coordinates

C	-0.202922	1.462679	0.034227
N	-1.441061	0.893181	0.083534
C	-1.755553	-0.513921	0.367065
N	-0.683661	-1.466752	0.160572
C	0.522719	-0.953170	0.073665
C	0.815006	0.423311	0.071880
N	1.709858	-1.672096	-0.045913
N	2.159644	0.522278	-0.050618
C	2.637272	-0.767710	-0.112316
H	3.695423	-0.966167	-0.204501
H	2.679061	1.383208	-0.107600
O	0.022208	2.652668	-0.075210
H	-2.233450	1.516390	0.050451
N	-2.946126	-0.823075	-0.390886
H	-3.292648	-1.730286	-0.101059
H	-2.695651	-0.901615	-1.371942
H	-2.020100	-0.604758	1.432384

Vibrational frequencies

65.0415	137.1808	174.0984
269.2482	283.2734	302.3727
359.8358	445.0662	523.8966
541.0073	569.7971	585.9507
637.9473	659.1870	715.3305
731.4363	781.1706	818.8813
903.4638	917.4447	938.0410

974.6100	1079.4740	1102.3261
1153.4651	1162.3498	1252.0893
1259.3239	1294.5340	1355.0822
1398.4753	1421.7426	1433.9086
1444.6003	1479.0908	1530.4946
1620.8895	1666.6980	1813.7778
2982.5597	3262.7398	3532.9745
3621.3468	3660.0738	3686.2654

i5

Cartesian coordinates

C	-0.336448	1.637484	0.039201
N	-1.534581	1.212485	0.214240
C	-1.766358	-0.223423	0.367081
N	-0.680623	-1.192206	0.315407
C	0.499340	-0.674364	0.139433
C	0.744292	0.715256	-0.007187
N	1.707050	-1.370010	0.051089
N	2.093433	0.829258	-0.186189
C	2.599100	-0.453085	-0.139753
H	3.658730	-0.632277	-0.257919
H	2.619723	1.672779	-0.334805
H	-0.175631	2.709360	-0.075454
N	-2.709450	-0.594840	-0.675503
H	-3.558705	-0.053107	-0.567422
H	-2.929905	-1.578744	-0.577641
H	-2.184577	-0.322030	1.387283

Vibrational frequencies

47.5766	185.1080	239.1392
272.9872	347.3061	427.0288
451.9985	467.3159	532.3061
587.8323	626.4195	683.0107
748.2647	766.3017	851.2200
872.3480	913.2600	927.1206
935.5492	981.8420	1023.5458
1100.9351	1128.0408	1198.2722
1264.0433	1275.2082	1324.5351
1340.0900	1379.1614	1405.4975
1424.4252	1457.6410	1536.1337
1615.9072	1626.5176	1650.3815
2912.7261	3135.4081	3254.4662
3544.9940	3640.9458	3700.5775

7H-purin-2-amine

Cartesian coordinates

C	0.273182	1.617909	-0.004864
N	1.517933	1.170411	-0.004159
C	1.704759	-0.170741	0.006355
N	0.770476	-1.120302	-0.001355
C	-0.474371	-0.655741	0.000992
C	-0.776768	0.717093	0.005315

N	-1.633373	-1.402278	-0.005428
N	-2.157673	0.779654	0.002907
C	-2.588335	-0.513857	-0.002777
H	-3.643826	-0.748548	-0.004250
H	-2.734538	1.601747	0.006392
H	0.132712	2.695873	-0.016832
N	3.006583	-0.580857	0.055995
H	3.704094	0.101031	-0.183662
H	3.183135	-1.544475	-0.167495

Vibrational frequencies

143.6888	212.6912	341.0412
365.8581	373.8451	434.0716
453.0498	475.9754	506.5446
541.9804	644.1971	644.5594
766.6165	813.1983	834.1483
846.9502	903.1597	952.5693
954.1999	995.6844	1124.0426
1130.4148	1205.8645	1281.4898
1318.0532	1354.6599	1403.7253
1438.3666	1488.3569	1530.1340
1562.4951	1642.1973	1654.1859
1706.9009	3172.0706	3250.3657
3645.7294	3716.9854	3775.8283

i6-complex

Cartesian coordinates

C	0.306511	1.288869	-0.844164
N	1.564259	0.960653	-0.613702
C	1.807408	-0.249797	-0.052244
N	0.918576	-1.184191	0.290425
C	-0.342604	-0.845945	0.050645
C	-0.708081	0.401139	-0.502234
N	-1.460107	-1.613009	0.276872
N	-2.077599	0.337767	-0.652424
C	-2.448850	-0.863759	-0.130910
H	-3.490075	-1.150613	-0.083070
H	-2.691862	1.110231	-0.841649
N	3.115520	-0.518112	0.208922
H	3.802392	0.071489	-0.225882
H	3.354312	-1.469107	0.427437
O	-0.889916	1.698144	1.548123
H	-0.081255	1.328148	1.930850
H	0.114966	2.259896	-1.289891

Vibrational frequencies

50.3134	85.5713	137.4017
150.7479	169.3609	207.6090
335.3551	346.9047	366.4961
440.9667	465.0916	486.2384
520.2349	543.0306	555.1450
629.4632	641.9451	763.0230

811.6339	826.9837	845.9232
916.7737	951.9698	969.3776
993.6371	1118.5105	1134.1226
1206.8686	1281.2812	1317.3803
1355.5483	1408.7896	1440.2653
1488.5287	1526.3407	1560.6488
1634.5339	1650.4033	1692.5530
3188.7963	3254.4804	3649.3254
3708.4742	3782.6000	3814.7542

i7

Cartesian coordinates

C	-0.296320	1.389360	0.386682
N	-1.582353	0.780913	0.210942
C	-1.689623	-0.498114	0.046139
N	-0.685361	-1.470313	-0.055043
C	0.531663	-0.957912	-0.002281
C	0.791984	0.406863	0.177132
N	1.726304	-1.651244	-0.150850
N	2.136674	0.531675	0.133669
C	2.642757	-0.739393	-0.073110
H	3.706169	-0.909337	-0.158629
H	2.654832	1.394050	0.160478
N	-2.931040	-1.053857	-0.041942
H	-3.707667	-0.429801	-0.170803
H	-2.985868	-1.985535	-0.413159
O	-0.119326	2.472882	-0.507529
H	-1.005004	2.810196	-0.664222
H	-0.240193	1.772336	1.421762

Vibrational frequencies

84.1037	144.3515	167.3457
199.1550	289.5177	325.3904
342.3018	379.1140	457.7379
511.5326	528.6081	545.0178
572.1265	630.2293	656.2229
719.3147	741.9411	823.2649
846.2903	883.7816	946.8622
976.7600	1035.8789	1084.2747
1099.5997	1165.9234	1234.5258
1266.8290	1281.8441	1328.6152
1365.9902	1411.6228	1423.2645
1439.2408	1502.9385	1540.8390
1602.8616	1619.3993	1680.4908
2932.9945	3264.0299	3644.5574
3692.3650	3778.3253	3884.9809

2-amino-7H-purin-6-ol

Cartesian coordinates

C	0.299659	1.291993	0.001022
N	1.521612	0.812382	0.000866
C	1.674432	-0.537560	0.006705

N	0.718771	-1.455515	-0.002423
C	-0.518255	-0.947400	0.000337
C	-0.785054	0.425309	0.006406
N	-1.699275	-1.654059	-0.006375
N	-2.159481	0.539806	0.003585
C	-2.630355	-0.736664	-0.003426
H	-3.691865	-0.940408	-0.005823
H	-2.697118	1.388190	0.007324
N	2.967411	-0.974266	0.055472
H	3.680606	-0.314875	-0.199882
H	3.115381	-1.943191	-0.166512
O	0.114344	2.617872	-0.006907
H	0.992404	3.014809	-0.003985

Vibrational frequencies

139.1120	173.8636	247.4776
297.8120	340.4110	362.4977
380.5595	450.5401	484.7616
510.6302	526.7320	564.9369
641.7906	643.6201	670.3984
709.8757	764.5426	820.8686
844.5311	894.6930	958.7830
1045.7147	1094.6899	1132.4234
1172.9988	1240.8509	1278.5384
1361.8080	1384.6188	1426.5575
1459.8995	1503.6096	1550.6853
1565.7784	1650.7320	1655.8667
1744.2040	3256.7927	3644.2089
3718.3391	3773.3993	3849.0748

Transition states

ts2a

Cartesian coordinates

C	-1.050122	0.778427	0.667684
N	-1.987980	-0.188893	0.520122
C	-1.607307	-1.364573	0.035870
N	-0.374281	-1.774324	-0.292602
C	0.563313	-0.857857	-0.110065
C	0.282683	0.425694	0.399300
N	1.914295	-0.981516	-0.372265
N	1.480787	1.071283	0.428433
C	2.408419	0.174804	-0.051581
H	3.451726	0.445291	-0.132640
H	1.643025	2.034579	0.666754
H	-2.396668	-2.097368	-0.098964
O	-1.259608	1.838554	-1.010055
H	-2.108951	1.438606	-1.241861
H	-1.323930	1.645649	1.254087

Vibrational frequencies

-481.4674	95.7842	111.1097
216.6679	251.9083	267.1534

429.9461	462.7028	512.0492
566.8847	612.6379	655.5428
667.3324	795.4957	810.8978
825.5297	914.8517	918.2506
937.7581	953.4530	992.5792
1102.8499	1132.2388	1206.7713
1277.4608	1296.5619	1335.6207
1385.2055	1424.2633	1447.3035
1492.5944	1547.6030	1610.3159
1657.1946	3193.1712	3212.9318
3261.6310	3704.3475	3824.3795

ts2b

Cartesian coordinates

C	1.177595	-0.642354	0.072650
N	1.946750	0.447742	-0.039414
C	1.344010	1.643363	-0.033207
N	0.046199	1.910360	-0.010245
C	-0.731797	0.821334	-0.010381
C	-0.218790	-0.480853	-0.017725
N	-2.108422	0.782097	-0.014212
N	-1.303569	-1.310995	-0.007015
C	-2.398881	-0.487542	-0.012951
H	-3.400223	-0.893510	-0.024517
H	-1.295000	-2.316115	-0.024729
H	2.012059	2.497976	-0.069277
O	1.728034	-1.853786	-0.127084
H	2.682058	-1.720350	-0.137875
H	1.077306	-0.665834	1.778957

Vibrational frequencies

-1187.2458	167.1429	204.4292
287.7174	302.2706	465.3233
483.7042	501.1203	509.7217
555.9094	595.4857	620.4328
645.7603	656.2112	718.7950
762.8200	840.0881	895.3405
902.0827	958.1563	999.6209
1083.8744	1114.4084	1166.8878
1270.0386	1303.5033	1336.8354
1361.8940	1401.6011	1432.9753
1440.4017	1506.8704	1555.5046
1609.5865	1688.5443	3197.9146
3264.9585	3706.6169	3850.4569

ts2c

Cartesian coordinates

C	-1.111520	-0.788212	0.000010
N	-1.904599	0.307504	0.000010
C	-1.418890	1.564776	0.000001
N	-0.145016	1.863683	-0.000008
C	0.684370	0.795180	-0.000008

C	0.260798	-0.541865	0.000001
N	2.054071	0.847060	-0.000016
N	1.408257	-1.296469	-0.000003
C	2.435096	-0.403757	-0.000013
H	3.464382	-0.732639	-0.000018
H	1.471058	-2.299832	0.000001
H	-2.146388	2.368492	0.000002
O	-1.884986	-1.801496	0.000020
H	-2.697288	-0.733223	0.000020

Vibrational frequencies

-1960.2644	160.2133	215.7519
284.9792	346.6948	498.4336
529.2799	570.0236	582.6807
632.9791	672.7980	689.2873
773.3919	811.3968	903.8869
945.5414	962.4760	985.1694
1108.1995	1124.9996	1150.7377
1220.5225	1302.6848	1349.1999
1386.1565	1420.5406	1433.6995
1484.3828	1541.0755	1574.5489
1613.8996	1745.9618	2142.5484
3219.7552	3259.7955	3707.4915

ts2d

Cartesian coordinates

C	0.320013	1.463284	-0.063026
N	1.503287	0.841661	-0.458971
C	1.678676	-0.525411	-0.623705
N	0.677865	-1.392869	-0.660997
C	-0.520020	-0.866237	-0.291412
C	-0.720838	0.473236	0.003960
N	-1.695603	-1.561188	-0.168265
N	-2.046975	0.591194	0.308681
C	-2.574637	-0.658966	0.187165
H	-3.620521	-0.852571	0.373937
H	-2.520211	1.443203	0.559819
O	0.234762	2.652348	0.162954
H	2.322343	1.431105	-0.467127
N	2.442198	-1.137989	1.162359
H	2.452196	-2.153945	1.029762
H	1.618340	-0.992317	1.755128
H	2.605186	-0.795362	-1.112701

Vibrational frequencies

-561.8471	103.5003	120.9094
169.1548	184.8730	237.1329
306.7749	327.8090	513.6498
544.0040	552.4815	554.1699
608.4181	630.2050	667.4770
689.9845	741.4356	755.5662
780.3864	802.8361	903.7375

910.9387	968.5945	990.0383
1101.7161	1112.3373	1140.9988
1237.6261	1311.7617	1340.1266
1411.2005	1427.9414	1454.9335
1497.2237	1524.8203	1558.2420
1560.7516	1618.1301	1829.9592
3228.1101	3265.2462	3430.5936
3524.5026	3653.7444	3694.7570

ts2e

Cartesian coordinates

C	-0.166114	1.452998	-0.010462
N	-1.432216	0.853472	-0.020881
C	-1.670784	-0.512731	0.084268
N	-0.728155	-1.428972	-0.035722
C	0.536417	-0.927090	-0.013328
C	0.833135	0.425836	-0.009596
N	1.688061	-1.666930	-0.020981
N	2.199144	0.505859	-0.013650
C	2.649946	-0.776726	-0.020393
H	3.705207	-1.006479	-0.024463
H	2.740739	1.353779	-0.011261
O	-0.014716	2.656426	-0.004453
H	-2.210848	1.480626	0.122692
N	-3.020861	-0.847277	-0.062545
H	-3.126175	-1.852479	-0.065344
H	-3.426019	-0.443431	-0.897116
H	-1.602588	-0.670209	1.804631

Vibrational frequencies

-1225.8435	142.5520	158.7713
187.9819	228.1334	302.9093
339.3922	371.7274	473.1747
521.5464	546.9330	571.1158
600.4624	621.6837	651.5933
662.9713	693.0461	710.4038
746.5660	800.9821	828.7957
839.1828	879.1421	968.7482
1044.1633	1107.5959	1139.9216
1176.8667	1224.2371	1304.4910
1324.3599	1403.6962	1428.6323
1470.0136	1502.8702	1554.5270
1581.1909	1618.0883	1663.1725
1831.9261	3263.9297	3570.0708
3642.3286	3669.0790	3699.8138

ts2f

Cartesian coordinates

C	-0.402783	1.613965	0.100689
N	-1.573918	1.149115	0.459604
C	-1.695982	-0.213622	0.599869
N	-0.686096	-1.116356	0.681663

C	0.478844	-0.629929	0.291538
C	0.662540	0.724627	-0.053502
N	1.674093	-1.317545	0.182331
N	1.989862	0.831108	-0.383403
C	2.523662	-0.422636	-0.223378
H	3.568099	-0.610934	-0.429112
H	2.477706	1.652639	-0.694973
H	-0.299012	2.686819	-0.041841
N	-2.366830	-0.646621	-1.226305
H	-3.319449	-0.281705	-1.124316
H	-2.469815	-1.657269	-1.088804
H	-2.614983	-0.521897	1.090518

Vibrational frequencies

-623.5194	90.5317	131.1400
195.1012	274.6168	288.8943
445.1624	463.2895	473.7519
570.8701	612.9259	661.6740
664.7716	780.7926	789.3168
815.4416	842.3538	907.5710
924.1977	946.2635	952.3584
972.2220	1114.7671	1116.4152
1203.5869	1259.9881	1301.6389
1325.6652	1375.5653	1424.3309
1437.7459	1496.5113	1537.0133
1556.9187	1604.2813	1655.1293
3166.4021	3173.2614	3253.8494
3414.6044	3519.7860	3707.1403

ts2g

Cartesian coordinates

C	-0.252576	1.625905	-0.039059
N	-1.492716	1.190507	-0.036273
C	-1.688292	-0.170601	0.065452
N	-0.737716	-1.134790	-0.023531
C	0.499875	-0.662163	-0.003326
C	0.795981	0.714229	0.010547
N	1.664476	-1.401779	-0.022438
N	2.172327	0.783563	0.001002
C	2.613205	-0.509272	-0.015944
H	3.670296	-0.735966	-0.020933
H	2.743876	1.609669	0.013609
H	-0.099747	2.700690	-0.097011
N	-2.984761	-0.579215	-0.192484
H	-3.684847	0.083390	0.099802
H	-3.168256	-1.531994	0.079022
H	-1.621742	-0.122389	1.735561

Vibrational frequencies

-1183.4535	139.8510	211.6955
320.8832	362.0498	425.7740
445.4833	458.7098	472.4243

520.4894	577.0321	593.6159
641.1876	651.4849	685.0574
770.4533	803.1572	835.8533
859.2850	902.5731	949.6884
957.5669	984.0593	1119.8601
1126.4937	1202.5028	1280.2910
1317.5434	1357.2826	1391.2919
1436.3296	1456.6764	1495.9274
1554.3673	1613.2877	1644.5282
1674.5909	3171.2960	3253.0317
3615.9134	3713.1695	3730.8498

ts2h

Cartesian coordinates

C	-0.266298	1.300241	0.651305
N	-1.534230	0.877230	0.542014
C	-1.748079	-0.355666	0.068464
N	-0.834830	-1.303498	-0.252504
C	0.413000	-0.916561	-0.083017
C	0.762868	0.374753	0.385186
N	1.554101	-1.661379	-0.309686
N	2.127185	0.374486	0.453193
C	2.527620	-0.857485	0.003270
H	3.577046	-1.108812	-0.062111
H	2.713714	1.176697	0.604197
N	-3.041923	-0.712688	-0.119697
H	-3.754960	-0.108267	0.246515
H	-3.242830	-1.680429	-0.296288
O	0.376850	2.182778	-1.046641
H	-0.235938	1.741862	-1.648278
H	-0.098620	2.225987	1.184613

Vibrational frequencies

-393.4377	98.8416	124.2783
152.0188	180.6551	234.5717
286.6386	344.7635	349.6360
435.9979	464.5750	491.8432
532.1976	552.1244	625.1313
635.0571	758.9029	781.0808
799.7436	830.4162	855.0225
912.6694	949.0621	969.9618
1007.3729	1098.5983	1112.1283
1197.1867	1288.9020	1322.2939
1348.0292	1407.2017	1425.6228
1479.5764	1501.3720	1549.8002
1608.9031	1652.8865	1672.6693
3230.7199	3257.3926	3652.1053
3708.2057	3789.7642	3843.6019

ts2i

Cartesian coordinates

C	-0.305197	1.289934	0.073575

N	-1.537059	0.787721	-0.029637
C	-1.674818	-0.551042	-0.003278
N	-0.705852	-1.472102	0.006096
C	0.525420	-0.963962	-0.007508
C	0.791788	0.412245	-0.012686
N	1.711005	-1.666220	-0.022170
N	2.156921	0.532047	-0.012509
C	2.637079	-0.747430	-0.024273
H	3.699621	-0.943685	-0.044015
H	2.688399	1.384492	-0.032559
N	-2.955700	-1.015313	0.023094
H	-3.686579	-0.364523	-0.201611
H	-3.087670	-1.986122	-0.199127
O	-0.129832	2.608262	-0.133584
H	-1.010247	2.998535	-0.134967
H	-0.095704	1.243803	1.771858

Vibrational frequencies

-1168.6042	136.2855	176.4783
229.1350	290.5655	338.4046
344.6915	359.8125	459.6642
473.1464	481.4378	490.9923
510.1678	558.8373	601.2874
638.1203	665.1066	680.0162
744.8392	762.8360	822.0422
847.4420	888.7778	955.9829
1046.8634	1082.9966	1120.3640
1165.3621	1225.8869	1277.9400
1347.4562	1389.2641	1418.8417
1441.4839	1489.4168	1515.1601
1563.6192	1625.0209	1649.9256
1696.8005	3260.2337	3646.9180
3713.9724	3778.5228	3856.6567

ts2j

Cartesian coordinates

C	0.278889	1.338166	-0.001042
N	1.491430	0.733176	-0.000107
C	1.639252	-0.614371	0.005838
N	0.626331	-1.458871	-0.000274
C	-0.591205	-0.885338	0.000513
C	-0.828274	0.498141	0.000729
N	-1.787640	-1.557162	-0.002271
N	-2.199430	0.643532	-0.001121
C	-2.699588	-0.617333	-0.002543
H	-3.765038	-0.798272	-0.003644
H	-2.715460	1.505617	0.000665
O	0.505089	2.593896	-0.000642
H	1.716286	2.012439	0.004834
N	2.907515	-1.103896	0.052866
H	2.999969	-2.085696	-0.143129
H	3.661647	-0.498312	-0.218200

Vibrational frequencies

-1888.5463	146.8743	148.9118
222.3513	326.0974	356.6994
360.8044	376.4255	464.7984
474.1550	500.0664	582.6712
617.1090	666.0551	673.1735
740.1275	746.5333	800.5259
849.2363	896.1906	959.3635
1086.8411	1091.9898	1134.6910
1143.2468	1195.8422	1289.3979
1335.6040	1397.9939	1414.7427
1476.2964	1508.6326	1554.2350
1577.9610	1630.3198	1661.8043
1755.2175	2156.1356	3260.8597
3642.3177	3713.8030	3768.8904

Product

guanine

Cartesian coordinates

C	-0.188180	1.443266	0.002776
N	-1.454912	0.826411	-0.006195
C	-1.680665	-0.533098	-0.004240
N	-0.748997	-1.431046	0.006390
C	0.518593	-0.922808	-0.001161
C	0.814930	0.429136	0.011011
O	-0.066657	2.650957	-0.005095
H	-2.232302	1.464628	-0.094668
N	1.669449	-1.660600	-0.006400
N	2.185414	0.510620	0.010088
C	2.633436	-0.769013	-0.000161
H	3.688110	-1.001745	-0.002927
H	2.727946	1.357334	0.015490
N	-3.002116	-0.911099	-0.067031
H	-3.117803	-1.903377	0.069723
H	-3.663260	-0.349386	0.445833

Vibrational frequencies

145.8780	156.8828	192.6909
303.2408	329.1697	342.8456
377.5552	493.0688	526.2549
545.5014	599.4146	602.9080
641.7474	657.8204	683.8638
742.5424	753.4980	806.5415
845.7686	877.1639	969.3176
1054.3113	1108.6352	1131.4903
1172.3471	1215.3722	1306.2778
1344.9483	1403.6108	1434.3410
1488.5563	1519.1675	1585.5725
1612.1902	1646.8836	1707.5010
1836.5021	3262.2788	3609.2158
3642.5547	3705.4295	3718.2112

***7H-purin-6-ol → ts2c → 1H-purin-6(7H)-one* pathway with H_2O solvent molecules**

7H-purin-6-ol + 1 H_2O

Cartesian coordinates

C	0.735747	-0.410588	-0.017101
N	1.303810	0.788327	-0.021437
C	0.506417	1.880709	-0.013025
N	-0.805859	1.927636	0.002480
C	-1.386492	0.716102	0.006613
C	-0.656067	-0.473797	-0.004465
N	-2.733734	0.443838	0.020169
N	-1.588303	-1.482023	0.002446
C	-2.802212	-0.860099	0.016350
H	-3.722173	-1.427149	0.023212
H	-1.406125	-2.470519	-0.007636
H	1.031168	2.830744	-0.019653
O	1.457826	-1.519330	-0.025706
H	3.240869	0.436022	-0.084969
O	3.856755	-0.318813	-0.051426
H	4.308121	-0.243218	0.790298
H	2.415731	-1.279147	-0.040038

Vibrational frequencies

55.8768	151.0961	175.1256
198.6896	219.7968	305.4025
315.0716	351.4122	396.5945
494.2272	539.3960	568.2203
591.1241	646.7424	650.7976
720.1661	735.3565	774.7500
826.7520	912.6685	912.6850
922.5599	963.8171	984.3058
1103.0735	1142.5798	1205.7226
1290.7742	1319.6609	1376.4847
1417.8463	1440.6888	1455.8254
1484.0951	1554.3709	1567.0578
1636.6800	1662.4535	1734.8546
3199.8984	3257.9468	3358.5355
3636.3338	3707.4669	3947.4202

ts2c + 1 H_2O

Cartesian coordinates

C	0.775213	-0.498660	-0.007809
N	1.346404	0.734685	-0.010376
C	0.591283	1.859534	-0.008393
N	-0.711111	1.933624	0.001127
C	-1.320922	0.725825	0.004674
C	-0.628182	-0.482377	-0.001458
N	-2.672588	0.495450	0.011963
N	-1.588746	-1.462172	0.002027
C	-2.782572	-0.808286	0.009304
H	-3.719531	-1.346324	0.012335

H	-1.429578	-2.454965	-0.006587
H	1.152136	2.788688	-0.015117
O	1.504721	-1.547933	-0.014241
H	2.649306	0.487123	-0.027687
O	3.522910	-0.296164	-0.070767
H	4.028335	-0.298458	0.744159
H	2.671650	-1.110613	-0.038133

Vibrational frequencies

-1575.9932	81.5587	179.5687
224.1293	248.3877	302.2791
409.9255	508.1287	513.2658
524.0354	564.8922	584.1343
638.6989	653.7263	679.7173
702.9021	737.9627	756.5055
820.7570	904.1460	935.6472
969.5307	981.6884	1109.5680
1149.9623	1215.2381	1236.8326
1313.9237	1340.7825	1378.6543
1408.0500	1431.9676	1444.7469
1491.8490	1513.9317	1545.3603
1584.2008	1613.3294	1713.5569
1747.2433	2012.7065	3198.9489
3263.9388	3703.5517	3926.2135

1H-purin-6(7H)-one + 1 H_2O

Cartesian coordinates

C	0.744600	-0.559697	-0.016107
N	1.270094	0.731495	-0.018338
C	0.521992	1.877287	-0.011687
N	-0.766361	1.937122	0.001602
C	-1.371434	0.712230	0.006217
C	-0.678328	-0.488387	-0.003212
N	-2.719066	0.483752	0.018570
N	-1.634781	-1.468239	0.003009
C	-2.830972	-0.822046	0.015875
H	-3.766871	-1.361074	0.022682
H	-1.466598	-2.460096	-0.005081
H	1.098423	2.796616	-0.018457
O	1.449816	-1.563714	-0.026706
H	2.293959	0.776811	-0.025535
O	3.903720	-0.247160	-0.050791
H	4.367206	-0.379019	0.776679
H	3.281241	-0.991485	-0.110724

Vibrational frequencies

54.1191	143.2877	166.7454
189.2009	200.7164	268.0113
286.7496	341.0758	380.7668
526.7651	539.9095	564.7468
576.8786	637.0347	656.4266
720.5339	735.7639	738.3597

813.3425	893.8442	915.1187
917.4568	969.5348	970.2648
1105.9243	1131.2840	1177.9982
1247.3259	1323.3284	1371.7690
1431.1256	1441.8271	1494.3627
1514.7524	1581.2066	1592.7107
1668.4684	1682.2366	1803.4067
3201.5207	3267.4957	3404.3324
3680.5050	3698.0734	3953.3644

7H-purin-6-ol + 2 H_2O

Cartesian coordinates

C	-0.260194	-0.462504	-0.009249
N	-0.861719	0.719763	0.059450
C	-0.095531	1.836210	0.122099
N	1.212326	1.928651	0.117543
C	1.831034	0.736944	0.039877
C	1.136113	-0.470309	-0.024356
N	3.185177	0.506811	0.013824
N	2.096963	-1.448706	-0.089040
C	3.292185	-0.792840	-0.063018
H	4.228353	-1.331023	-0.104229
H	1.941618	-2.440160	-0.148043
H	-0.652951	2.766337	0.184425
O	-0.917078	-1.599096	-0.066530
H	-2.641534	1.107095	-0.062408
O	-3.525457	-1.457848	0.133553
H	-3.852926	-1.667327	1.008729
H	-1.908542	-1.489343	-0.001873
O	-3.613838	1.183231	-0.178977
H	-3.775479	-0.521035	-0.024500
H	-3.738420	1.534525	-1.061031

Vibrational frequencies

33.9891	49.8324	95.0945
176.7250	182.9394	199.8244
222.3729	262.5935	282.9340
310.8502	369.7248	378.1763
411.1751	502.8682	523.1395
545.5671	572.6195	593.8638
648.9085	654.9269	724.3080
742.3226	793.4933	830.2708
907.7742	913.5223	965.3914
985.7906	1012.0798	1045.7753
1107.1731	1147.0512	1207.1504
1292.2251	1323.7228	1379.7456
1418.1186	1445.2468	1455.3893
1479.0820	1557.3516	1564.8202
1633.2221	1676.5810	1684.6393
1727.2718	3125.9579	3187.9363
3261.4510	3430.2199	3517.0988
3708.5508	3950.4859	3952.5493

ts2c + 2 H_2O

Cartesian coordinates

C	-0.340772	-0.447667	-0.035237
N	-0.865216	0.803945	0.008541
C	-0.054761	1.892909	0.070340
N	1.248676	1.929941	0.086982
C	1.813942	0.701118	0.033535
C	1.069384	-0.469898	-0.026996
N	3.155660	0.413493	0.034157
N	1.985813	-1.490836	-0.062345
C	3.207910	-0.892844	-0.024404
H	4.120296	-1.471434	-0.042455
H	1.778467	-2.473323	-0.111971
H	-0.582171	2.842196	0.111523
O	-1.041842	-1.506247	-0.080648
H	-2.232386	1.010446	-0.054896
O	-3.442927	-1.327241	0.105711
H	-3.724763	-1.632076	0.969462
H	-2.337556	-1.447527	0.015335
O	-3.351692	1.042118	-0.091197
H	-3.545596	-0.166199	0.013364
H	-3.633353	1.371365	-0.946073

Vibrational frequencies

-1269.3479	53.2913	63.1520
125.6018	179.0572	223.3124
263.4498	306.5227	339.8288
420.6135	478.9806	517.1784
537.8161	578.6236	589.1760
616.0886	632.1401	656.0728
660.6792	716.4899	735.8287
743.5329	762.0335	827.9143
902.6236	938.8026	972.9898
978.1597	1106.8319	1151.0023
1171.1934	1236.4706	1303.9718
1323.6407	1382.9831	1406.0360
1431.9710	1449.0502	1486.0152
1511.7041	1546.4203	1568.7566
1597.8265	1614.8012	1657.6012
1686.3152	1719.8034	1819.3985
1881.9616	3182.7625	3256.5841
3708.1229	3935.0690	3937.1980

1H-purin-6(7H)-one + 2 H_2O

Cartesian coordinates

C	-0.289697	-0.495296	-0.094006
N	-0.766695	0.805411	-0.034143
C	0.028247	1.914305	0.071110
N	1.318300	1.924902	0.120605
C	1.875058	0.680758	0.055766
C	1.133227	-0.485789	-0.048238

N	3.211929	0.394320	0.085409
N	2.048138	-1.504793	-0.081066
C	3.269097	-0.912085	0.001169
H	4.181604	-1.490027	-0.005146
H	1.839518	-2.486021	-0.155772
H	-0.515916	2.851961	0.116176
O	-1.017691	-1.484324	-0.174531
H	-1.791022	0.951742	-0.076878
O	-3.728519	-1.442251	0.204704
H	-3.849209	-1.827066	1.072733
H	-2.781058	-1.565887	-0.000369
O	-3.523681	1.214790	-0.107558
H	-3.790718	0.289151	0.076595
H	-3.911367	1.420202	-0.958683

Vibrational frequencies

32.3553	55.9629	73.8394
163.5298	180.5526	199.7253
210.0935	252.5119	281.7345
290.4194	343.5048	362.0426
393.2880	507.0422	536.2298
536.4038	568.8190	579.5652
634.6238	657.6347	727.0730
740.2352	753.3421	817.8550
898.9142	915.2018	954.9260
963.7148	969.7412	1030.3411
1105.7202	1137.4164	1188.6160
1248.0863	1323.3079	1373.8607
1431.4353	1443.2181	1498.1974
1536.6569	1587.2140	1598.8656
1674.5808	1684.9327	1696.0349
1790.4216	3205.6466	3209.7299
3261.4130	3496.6663	3594.9988
3700.7743	3951.8278	3960.9561

7H-purin-6-ol + 3 H_2O

Cartesian coordinates

C	-0.202352	-0.504728	-0.234831
N	0.433028	0.662641	-0.287018
C	-0.283506	1.801537	-0.125391
N	-1.571784	1.935621	0.071583
C	-2.227848	0.761193	0.115485
C	-1.584120	-0.466239	-0.031920
N	-3.574198	0.570758	0.308929
N	-2.567732	-1.417159	0.077967
C	-3.725673	-0.726853	0.278958
H	-4.670073	-1.237968	0.399443
H	-2.447373	-2.413741	0.022212
H	0.302443	2.715829	-0.165645
O	0.403896	-1.658271	-0.369175
H	2.133004	1.013752	-0.621286
O	2.990212	-1.564504	-0.512372

H	3.236645	-0.811385	-1.064614
H	1.404716	-1.578214	-0.435935
O	3.095801	1.188949	-0.767412
H	3.808636	0.664586	0.875236
H	3.158403	1.982012	-1.298058
O	3.995498	-0.025807	1.532706
H	3.350931	-1.295074	0.353458
H	4.945214	-0.015222	1.651177

Vibrational frequencies

27.6419	33.6660	70.1284
87.6153	168.0710	180.2434
181.3105	192.9829	226.9999
227.7891	249.2248	273.5956
299.0545	312.6708	369.5837
383.0310	469.1676	506.9786
536.6916	555.3641	574.4795
593.1440	625.1117	651.9859
667.0362	727.3471	738.2596
746.2931	831.8467	859.7260
914.9342	917.9356	935.3347
966.4704	982.2698	1108.9877
1134.5175	1148.8029	1207.8110
1294.8603	1326.5564	1379.8232
1419.8566	1446.3484	1459.4514
1481.2063	1558.3807	1566.5636
1631.9941	1665.7253	1697.4069
1722.8770	1736.0587	3002.8314
3177.2964	3260.5428	3308.9440
3618.6281	3697.5151	3708.7211
3824.6791	3958.7878	3968.9743

ts2c + 3 H_2O

Cartesian coordinates

C	0.111613	-0.443759	0.136900
N	-0.401243	0.813443	0.141769
C	0.417126	1.892949	0.034748
N	1.717547	1.924872	-0.071539
C	2.273012	0.689783	-0.074836
C	1.521511	-0.472275	0.022934
N	3.609098	0.387777	-0.177139
N	2.426042	-1.503945	-0.022408
C	3.649463	-0.919907	-0.142542
H	4.553501	-1.508955	-0.201029
H	2.207128	-2.484221	0.015580
H	-0.106050	2.846103	0.039371
O	-0.579211	-1.498850	0.224087
H	-1.758793	1.205278	0.275710
O	-2.990358	-1.859271	0.168085
H	-3.231586	-2.067535	1.070906
H	-1.942899	-1.647982	0.166110
O	-2.769200	1.617100	0.358874

H	-3.596394	0.822010	-0.269271
H	-2.950024	1.761288	1.287750
O	-4.128170	0.005938	-0.788634
H	-3.656044	-0.942652	-0.336186
H	-5.079781	0.061553	-0.706247

Vibrational frequencies

-970.5073	27.7505	37.8491
73.6042	87.4741	112.3992
176.7733	223.2416	242.9118
278.2119	305.3561	368.7605
405.3598	423.0408	434.0865
515.3819	568.8864	575.7497
591.1640	614.0966	631.3055
655.3784	657.2833	681.7166
700.5084	745.6422	753.3283
800.8527	831.8733	895.3761
934.9442	971.9177	983.7549
1103.8133	1149.4859	1191.7030
1219.3209	1252.9417	1266.9965
1327.3163	1381.4988	1396.0159
1409.2094	1436.4348	1450.4209
1497.9731	1531.6674	1560.5001
1603.8299	1612.7915	1674.3254
1698.2908	1705.0582	1771.4511
1823.6776	1972.6792	2133.9301
3178.7601	3256.1645	3710.9771
3948.5525	3952.1097	3960.1120

1H-purin-6(7H)-one + 3 H_2O

Cartesian coordinates

C	-0.207520	-0.572094	-0.209414
N	0.330491	0.702465	-0.242331
C	-0.396946	1.854096	-0.107314
N	-1.675154	1.931407	0.059921
C	-2.291036	0.714542	0.099871
C	-1.616579	-0.490347	-0.025529
N	-3.630360	0.494614	0.269439
N	-2.575020	-1.464105	0.072211
C	-3.754006	-0.809638	0.247305
H	-4.687583	-1.342031	0.355225
H	-2.417623	-2.456596	0.027202
H	0.201475	2.757816	-0.149931
O	0.460256	-1.599702	-0.327117
H	1.345828	0.830599	-0.376388
O	3.160949	-1.926915	-0.280556
H	3.354700	-1.986739	-1.215410
H	2.187280	-1.847146	-0.234070
O	2.886281	1.686608	-0.512446
H	3.497285	1.259079	0.125326
H	3.345628	1.677565	-1.351545
O	4.295768	0.094920	1.086151

H	3.971765	-0.727908	0.665207
H	5.222054	-0.033956	1.281938

Vibrational frequencies

24.4012	32.0163	45.6464
54.7151	68.0760	161.7733
173.1031	177.1349	195.6693
202.9281	221.2268	278.0604
290.8073	296.0347	313.6502
349.5527	389.9998	456.2710
485.4497	536.4804	536.9573
569.7322	582.9504	634.3119
658.3591	732.8828	742.0559
762.4070	819.9862	834.1409
899.7937	914.8439	940.4321
969.9187	977.1293	1063.7052
1108.0965	1138.8007	1180.1000
1244.4275	1325.9721	1366.7639
1425.1824	1442.7083	1494.2185
1519.0431	1584.9977	1594.0097
1661.6890	1681.6590	1686.4994
1697.6317	1784.2654	3209.5851
3266.3968	3273.2912	3470.1752
3538.3120	3587.1283	3701.2409
3962.0847	3964.9874	3979.3607

***2-amino-7H-purin-6-ol → ts2j → guanine* pathway with H_2O solvent molecules**

2-amino-7H-purin-6-ol + 1 H_2O

Cartesian coordinates

C	0.488519	-0.798598	-0.054980
N	1.263434	0.277019	-0.051388
C	0.671061	1.500621	-0.013298
N	-0.622945	1.766834	0.021525
C	-1.399097	0.675025	0.024313
C	-0.890552	-0.624380	-0.015388
N	-2.773090	0.641826	0.056893
N	-1.989397	-1.456696	-0.006027
C	-3.069585	-0.632125	0.037149
H	-4.075111	-1.028172	0.053547
H	-1.985948	-2.461050	-0.030119
O	1.008891	-2.015910	-0.096035
H	3.080022	-0.405853	-0.006981
O	3.588980	-1.237510	0.029364
H	3.951674	-1.273392	0.915650
H	1.992000	-1.947973	-0.088928
N	1.534005	2.564389	0.027069
H	2.456260	2.410912	-0.342089
H	1.112022	3.456022	-0.170990

Vibrational frequencies

54.0720	136.2325	143.2442

183.3183	199.3435	240.0611
324.6579	334.5686	369.9063
373.4463	396.8219	427.9507
461.8377	503.1889	515.0292
572.7058	641.0182	642.1651
700.2149	714.0916	764.8551
795.5482	821.5577	849.2322
898.2437	907.9046	960.4483
1072.6398	1101.1802	1135.6820
1178.8083	1256.0476	1315.2111
1387.3112	1417.0622	1443.5100
1473.9703	1521.7004	1551.1554
1561.7305	1650.4687	1653.9318
1661.2001	1744.9319	3259.9769
3404.2315	3613.3053	3635.8608
3714.3762	3758.1736	3943.1908

ts2j + 1 H_2O

Cartesian coordinates

C	0.466920	-0.904058	-0.029744
N	1.290657	0.177939	-0.021137
C	0.794058	1.445553	-0.003650
N	-0.475444	1.780020	0.011819
C	-1.317597	0.727925	0.014673
C	-0.898533	-0.600841	-0.011122
N	-2.687626	0.788101	0.032427
N	-2.049819	-1.356852	-0.008133
C	-3.072272	-0.464615	0.017933
H	-4.103007	-0.789086	0.025577
H	-2.107534	-2.360016	-0.026065
O	0.969133	-2.080843	-0.050149
H	2.486879	-0.326120	0.004368
O	3.205820	-1.279950	-0.023762
H	3.652861	-1.402342	0.815655
H	2.181467	-1.899454	-0.040033
N	1.730596	2.444567	0.040297
H	2.635266	2.242700	-0.350456
H	1.360429	3.360460	-0.153194

Vibrational frequencies

-1609.3396	77.5198	146.7048
189.1807	227.9356	232.4802
321.3899	373.4681	402.3759
434.7968	480.1761	500.4296
520.9938	527.8269	580.1357
624.8637	647.4749	652.2245
686.6265	733.2517	751.2454
756.7139	814.6907	856.6875
896.0204	964.4628	1103.1345
1131.1577	1136.6557	1183.7387
1203.2595	1257.6517	1318.8125
1394.7209	1415.5613	1434.9240

1473.9376	1502.5797	1511.0287
1554.9175	1580.9021	1626.4825
1658.9455	1718.1989	1742.8038
1995.2123	3256.7436	3629.3527
3711.9776	3748.3277	3924.8207

guanine + 1 H_2O

Cartesian coordinates

C	0.463211	-0.942170	-0.037071
N	1.211659	0.236840	-0.024871
C	0.678665	1.503318	-0.007687
N	-0.591620	1.771940	0.007419
C	-1.391634	0.671034	0.015874
C	-0.921600	-0.633481	-0.013786
N	-2.759062	0.680469	0.040024
N	-2.039263	-1.433303	-0.006638
C	-3.098308	-0.587442	0.026191
H	-4.114810	-0.952838	0.039159
H	-2.050163	-2.438554	-0.023735
O	0.998110	-2.047821	-0.061338
H	2.224691	0.090155	0.014130
O	3.636933	-1.180593	-0.008081
H	4.021189	-1.407230	0.839439
H	2.885578	-1.791484	-0.109526
N	1.593027	2.523297	0.042384
H	2.485283	2.375096	-0.400332
H	1.182694	3.429902	-0.113134

Vibrational frequencies

55.6529	131.6012	148.7448
167.9876	188.7697	200.0381
296.5755	328.0088	360.3194
373.9097	377.1661	385.3178
499.3627	512.3527	552.3535
560.9038	645.4844	651.1060
696.8564	732.7765	742.9455
743.9140	807.1667	846.8217
877.5824	884.5718	967.5084
1071.8929	1112.6538	1139.5203
1181.4457	1227.9278	1310.6884
1391.6824	1414.1625	1441.2792
1495.4442	1528.5014	1591.2969
1613.3131	1653.1421	1673.0230
1708.4687	1801.3794	3263.6504
3401.2796	3621.3522	3654.5051
3706.1413	3735.8943	3949.8011

2-amino-7H-purin-6-ol + 2 H_2O

Cartesian coordinates

C	-0.117763	-0.752943	-0.035677
N	-0.832166	0.363094	0.008482
C	-0.180718	1.559018	0.072162

N	1.123411	1.761623	0.089765
C	1.843777	0.632304	0.024030
C	1.270249	-0.637841	-0.041082
N	3.214409	0.530396	0.023242
N	2.325708	-1.523595	-0.078644
C	3.446524	-0.755998	-0.040173
H	4.431122	-1.201047	-0.062605
H	2.269664	-2.525191	-0.134015
O	-0.682872	-1.941512	-0.078393
H	-2.572070	0.568417	-0.228401
O	-3.319347	-1.949286	0.221975
H	-3.576826	-2.116836	1.129039
H	-1.673025	-1.896080	0.004313
O	-3.550339	0.689789	-0.273594
H	-3.647602	-1.049679	0.019629
H	-3.732160	0.976792	-1.169335
N	-0.997153	2.659252	0.082085
H	-1.945360	2.528084	0.395499
H	-0.545159	3.520972	0.335911

Vibrational frequencies

46.4540	48.7249	98.7414
145.2245	184.2048	189.3638
200.4631	239.1666	263.0635
269.6262	346.3940	359.7249
369.0798	382.3306	398.6751
466.3131	477.4239	497.6773
512.7414	519.4586	576.8775
642.1165	648.2733	706.4624
717.4570	765.3629	821.9151
822.8978	851.6865	897.6834
962.5592	996.1658	1063.7990
1079.3639	1108.3804	1142.4847
1185.2889	1265.1343	1319.3434
1389.0885	1413.1559	1439.4421
1480.3407	1511.2642	1564.3131
1564.8394	1650.7997	1659.7278
1667.2371	1680.9107	1739.5014
3230.7498	3262.1002	3349.7491
3563.6720	3618.7989	3715.7990
3745.2322	3944.7059	3953.9580

ts2j + 2 H_2O

Cartesian coordinates

C	-0.203292	-0.753419	-0.045369
N	-0.848874	0.438220	-0.022338
C	-0.159474	1.617374	0.039879
N	1.142711	1.765972	0.070280
C	1.817029	0.598360	0.020282
C	1.196646	-0.645157	-0.036961
N	3.180104	0.445538	0.033817
N	2.215698	-1.571149	-0.055144

C	3.365369	-0.851314	-0.014339
H	4.332630	-1.332858	-0.022733
H	2.113474	-2.569776	-0.102502
O	-0.815287	-1.870395	-0.074566
H	-2.131277	0.517291	-0.138632
O	-3.205314	-1.832335	0.168051
H	-3.455887	-2.103303	1.052079
H	-2.051976	-1.880009	0.049121
O	-3.316236	0.526176	-0.173022
H	-3.412121	-0.714492	0.015838
H	-3.616404	0.761058	-1.052359
N	-0.949572	2.738003	0.031104
H	-1.893146	2.637635	0.369891
H	-0.468741	3.585742	0.280611

Vibrational frequencies

-1475.0351	52.8221	69.5722
108.3544	149.9853	185.1827
232.7516	264.9784	316.8443
371.6675	391.0508	399.4939
448.0964	485.6190	487.1152
511.0822	547.3546	577.3097
612.3557	617.6289	631.2236
650.2326	698.7254	732.4367
736.3062	757.9807	760.6434
817.8314	864.8919	891.9448
969.3218	988.9680	1101.5276
1118.2906	1148.2883	1187.8741
1272.0175	1328.8221	1385.8051
1402.4334	1426.9066	1451.3370
1476.6291	1514.4041	1522.8509
1563.0336	1574.6310	1610.9850
1635.3895	1660.9188	1680.2600
1725.1879	1755.6008	1857.2018
3264.2726	3616.9773	3713.0804
3740.9696	3930.7734	3940.6054

guanine + 2 H_2O

Cartesian coordinates

C	-0.079966	-0.878462	-0.196561
N	-0.776136	0.321207	-0.170124
C	-0.206338	1.562825	0.000316
N	1.070759	1.778881	0.125347
C	1.826129	0.650626	0.067234
C	1.310781	-0.630061	-0.088478
N	3.190108	0.599107	0.170866
N	2.396335	-1.474558	-0.072792
C	3.481620	-0.677264	0.080217
H	4.481459	-1.084373	0.120911
H	2.372394	-2.474807	-0.170160
O	-0.652079	-1.965695	-0.300143
H	-1.794675	0.294140	-0.266063

O	-3.303082	-1.930910	0.386549
H	-3.303642	-2.306951	1.266661
H	-2.390759	-2.063093	0.054554
O	-3.587352	0.692937	-0.121402
H	-3.680317	-0.236874	0.178257
H	-4.055864	0.733711	-0.955784
N	-1.094611	2.594865	-0.000339
H	-2.063346	2.388405	0.196175
H	-0.723682	3.476684	0.308351

Vibrational frequencies

37.3344	61.3287	62.9485
151.5226	160.4741	176.2909
186.5333	204.3691	259.4739
287.0687	334.1688	343.8243
361.1297	374.4846	407.3655
460.3073	492.5254	503.0219
505.9640	552.0332	558.7197
648.9391	653.0404	697.0365
736.6230	745.5646	794.7996
808.8274	845.1499	882.1701
887.0912	965.7045	968.1064
1079.1515	1116.4358	1149.8321
1183.9520	1237.1557	1315.9909
1388.5417	1411.3568	1440.6218
1492.2793	1527.0128	1600.4274
1609.7321	1650.9862	1678.3437
1700.2629	1716.9435	1782.1304
3263.8165	3385.1688	3491.5010
3556.3686	3599.9441	3708.2584
3743.5100	3949.2847	3957.8858

2-amino-7H-purin-6-ol + 3 H_2O

Cartesian coordinates

C	-0.300121	-0.766390	-0.112718
N	0.421678	0.347835	-0.137313
C	-0.217121	1.544250	-0.017396
N	-1.511493	1.758953	0.097356
C	-2.244703	0.633659	0.094366
C	-1.683795	-0.638881	0.001933
N	-3.611135	0.541213	0.198220
N	-2.742515	-1.518487	0.054188
C	-3.853879	-0.744862	0.169403
H	-4.839080	-1.184635	0.231330
H	-2.693447	-2.521350	0.014090
O	0.246682	-1.956094	-0.200349
H	2.075937	0.570183	-0.708643
O	2.859878	-1.957368	-0.336949
H	3.105590	-1.334075	-1.030493
H	1.246232	-1.918693	-0.234949
O	3.004434	0.774917	-0.983588
H	3.913632	0.427861	0.590647

H	2.934729	1.485621	-1.621262
O	4.118135	-0.154988	1.340201
H	3.277412	-1.556335	0.447683
H	5.072917	-0.219089	1.363256
N	0.612125	2.646288	-0.064857
H	0.156241	3.495323	0.229120
H	1.533891	2.506176	0.318015

Vibrational frequencies

27.5990	31.0746	66.9838
90.1434	146.1670	155.8783
178.3571	188.5244	192.4480
225.5901	246.9836	265.9698
273.7399	309.0951	343.1222
369.8606	375.6704	389.2028
423.1965	475.9863	492.1414
512.6124	535.0386	576.0128
593.9720	625.7216	645.6453
650.1309	709.7022	723.5126
738.3221	774.5743	826.9622
852.1099	860.9931	904.5813
963.7706	970.2247	1072.6503
1110.3392	1111.6808	1146.9471
1187.5355	1265.6416	1320.8072
1387.9170	1414.3292	1440.2568
1481.3940	1503.8659	1560.7212
1565.6568	1645.7854	1651.5288
1665.8761	1706.8759	1723.7533
1739.0088	3103.5863	3258.5474
3298.5799	3609.8504	3627.5764
3698.3253	3713.4354	3724.5774
3852.8436	3954.2374	3959.7615

ts2j + 3 H_2O

Cartesian coordinates

C	0.201753	-0.763361	0.222330
N	-0.430610	0.436240	0.255708
C	0.231750	1.640211	0.088723
N	1.527158	1.762632	-0.087855
C	2.192278	0.593085	-0.100864
C	1.583324	-0.652907	0.048390
N	3.542789	0.433984	-0.274576
N	2.597419	-1.581492	-0.044181
C	3.731228	-0.862951	-0.233741
H	4.692518	-1.345082	-0.339004
H	2.501794	-2.580326	0.013339
O	-0.404240	-1.876612	0.340147
H	-1.496097	0.552121	0.401512
O	-2.784636	-2.075043	0.304245
H	-3.138090	-1.915765	1.180263
H	-1.584777	-1.927776	0.320911
O	-2.876482	1.221169	0.396849

H	-3.477657	0.436019	-0.477512
H	-3.348974	1.307362	1.224061
O	-3.776418	-0.400051	-1.130670
H	-3.289846	-1.393127	-0.383576
H	-4.714846	-0.382948	-1.310848
N	-0.568320	2.719796	0.133192
H	-0.151980	3.605474	-0.088152
H	-1.578890	2.565772	0.149381

Vibrational frequencies

-930.6066	37.7884	49.8812
78.7741	108.0293	141.6212
149.6931	187.3655	227.4765
253.4512	305.7685	359.3873
368.6140	382.1420	384.6907
411.1517	461.5472	475.5520
478.2319	503.2594	549.6990
564.6953	587.8019	594.0612
643.3919	698.8151	706.5196
723.5964	734.6539	752.6772
774.5709	812.4700	817.9147
843.5844	915.6077	965.2132
1070.8106	1119.4055	1138.9806
1163.5682	1193.7998	1235.4571
1262.5884	1324.5540	1390.0481
1414.1463	1421.4625	1433.1370
1451.7277	1484.6473	1517.4109
1551.5083	1587.2966	1623.2020
1646.8701	1670.7843	1708.2856
1743.0874	1767.5124	1813.5933
1985.8826	2515.2254	3256.6988
3411.6968	3713.3078	3743.7155
3944.3588	3950.9094	3967.3903

guanine + 3 H_2O

Cartesian coordinates

C	-0.291061	-0.817092	-0.242639
N	0.319007	0.429046	-0.263836
C	-0.342502	1.630651	-0.091462
N	-1.626449	1.743406	0.106768
C	-2.290220	0.560898	0.125796
C	-1.684699	-0.676622	-0.041774
N	-3.637125	0.402982	0.317966
N	-2.695085	-1.605725	0.054680
C	-3.828848	-0.894455	0.267883
H	-4.787940	-1.378264	0.382542
H	-2.593580	-2.603264	-0.015893
O	0.339299	-1.867695	-0.384656
H	1.331143	0.472621	-0.401190
O	3.009902	-2.240338	-0.291296
H	3.221619	-2.331393	-1.219616
H	2.034078	-2.148037	-0.264784

O	2.991711	1.443029	-0.429394
H	3.548415	0.928499	0.198683
H	3.472661	1.466396	-1.255983
O	4.208114	-0.306804	1.119629
H	3.845648	-1.102733	0.675086
H	5.110594	-0.502884	1.364337
N	0.439580	2.734072	-0.168709
H	0.003929	3.594719	0.110629
H	1.445695	2.632057	-0.122987

Vibrational frequencies

27.4647	34.9203	51.8325
67.6430	103.6822	149.1215
164.3456	172.3378	187.3169
195.7343	206.8633	219.9298
287.4642	313.2369	321.6102
351.3521	367.9933	377.6021
390.3113	412.2776	478.0100
498.9563	501.4800	506.8791
555.5293	639.6103	655.8373
659.0080	699.1372	741.4895
747.2495	780.1152	810.4279
844.8971	852.5753	901.8132
908.8225	968.0555	999.3415
1065.0124	1119.6575	1151.6594
1187.5469	1240.0249	1317.6989
1384.0715	1411.3030	1440.5864
1490.5163	1525.7705	1602.0017
1613.5292	1645.5231	1665.0019
1687.2935	1700.8996	1711.3845
1782.3715	3257.4061	3391.2871
3455.6943	3487.4465	3546.3237
3565.3067	3712.4671	3743.7217
3964.3864	3965.4059	3983.9509

2) SCRF/PCM//ωB97X-D/6-311G(d,p) for *7H-purin-6-ol → ts2c → 1H-purin-6(7H)-one* pathway with H_2O solvent molecules

7H-purin-6-ol + 0 H_2O

Cartesian coordinates

C	-1.175374	-0.666258	0.000144
N	-1.960343	0.394019	0.000047
C	-1.386235	1.613459	-0.000090
N	-0.099982	1.905063	-0.000098
C	0.696362	0.822041	-0.000113
C	0.205398	-0.486391	0.000026
N	2.069881	0.811157	0.000098
N	1.313258	-1.295400	-0.000149
C	2.384513	-0.463330	0.000065
H	3.391477	-0.853567	0.000124
H	1.337091	-2.302271	-0.000292
H	-2.079376	2.448787	0.000002

O	-1.699572	-1.889272	0.000079
H	-2.660306	-1.799777	0.000062

Vibrational frequencies

170.1227	217.7042	296.7502
313.4152	508.6771	535.6512
538.6565	552.7879	593.1028
627.0534	654.5980	717.8965
737.1768	831.2902	905.7008
926.6372	962.3771	999.4810
1100.1764	1140.3592	1180.5712
1274.9553	1311.2113	1352.9247
1374.8251	1408.6868	1437.8529
1464.2198	1545.4385	1548.8280
1628.8360	1719.1499	3197.8674
3275.2506	3690.9281	3832.7351

ts2c + 0 H_2O

Cartesian coordinates

C	-1.105375	-0.790256	0.000010
N	-1.902810	0.302510	0.000010
C	-1.428740	1.559983	0.000001
N	-0.151882	1.862817	-0.000008
C	0.680705	0.794707	-0.000008
C	0.266074	-0.545668	0.000001
N	2.047969	0.856002	-0.000016
N	1.418543	-1.289468	-0.000003
C	2.437276	-0.400402	-0.000013
H	3.465829	-0.728899	-0.000018
H	1.497460	-2.293777	0.000001
H	-2.160798	2.358872	0.000002
O	-1.886166	-1.803348	0.000020
H	-2.695541	-0.742613	0.000020

Vibrational frequencies

-2000.9528	161.2438	217.2139
286.3828	350.9783	529.4413
541.9844	569.9270	583.6566
639.3476	672.8328	689.4972
774.4353	813.3489	929.4955
946.8980	964.4069	990.8260
1106.4758	1119.9788	1160.0720
1221.9141	1296.8200	1353.1837
1386.8949	1420.2210	1432.3010
1482.3110	1535.2697	1566.2322
1601.1780	1722.4478	2131.8651
3226.2933	3273.1873	3687.2362

1H-purin-6(7H)-one + 0 H_2O

Cartesian coordinates

C	-1.120380	0.906765	-0.000234
N	-1.929174	-0.236691	0.000041

C	-1.482412	-1.527843	0.000046
N	-0.240805	-1.885079	-0.000057
C	0.634051	-0.832234	-0.000011
C	0.250277	0.498802	0.000053
N	1.996608	-0.935905	-0.000184
N	1.416410	1.216818	0.000190
C	2.420939	0.311145	-0.000032
H	3.456476	0.615695	-0.000052
H	1.508233	2.220310	0.000463
H	-2.262016	-2.280867	0.000131
O	-1.586514	2.032902	0.000062
H	-2.926708	-0.072168	0.000102

Vibrational frequencies

160.4190	195.4053	285.1807
311.1843	524.0451	556.7424
560.5550	571.0180	622.2082
651.7761	689.0161	723.6814
758.3035	818.4561	907.6058
917.5150	970.9654	976.9766
1107.2112	1135.8426	1159.9677
1227.1108	1311.7915	1374.1265
1427.4125	1440.5611	1475.3254
1500.3714	1578.6151	1591.9236
1673.8060	1788.5624	3224.9220
3272.7281	3636.0856	3681.4432

7H-purin-6-ol + 1 H_2O

Cartesian coordinates

C	0.733204	-0.405875	-0.023995
N	1.295649	0.798062	-0.028622
C	0.500356	1.886547	-0.014945
N	-0.815994	1.928132	0.003040
C	-1.390518	0.711100	0.006857
C	-0.659490	-0.478025	-0.006811
N	-2.735968	0.439097	0.024841
N	-1.592637	-1.483986	0.002989
C	-2.802479	-0.872765	0.021557
H	-3.717621	-1.445972	0.032151
H	-1.421473	-2.476521	-0.002292
H	1.022849	2.837756	-0.018730
O	1.470222	-1.501361	-0.038370
H	3.288867	0.451269	-0.041069
O	3.874035	-0.325896	-0.044034
H	4.303203	-0.320612	0.814843
H	2.426333	-1.242890	-0.037390

Vibrational frequencies

51.3892	126.9011	170.7312
190.5880	221.3939	303.5361
318.4628	352.1741	387.8593
536.4701	538.0558	566.2361

590.2881	641.4463	653.0267
688.8280	720.5877	748.2680
828.7420	904.5341	913.4525
936.5538	964.9937	988.3391
1114.9081	1151.9661	1206.4352
1288.6093	1331.0184	1374.4311
1411.1282	1436.5152	1452.5936
1480.6489	1548.0630	1559.9260
1626.1511	1646.7754	1723.9736
3200.4506	3270.8382	3288.9865
3664.7542	3685.8835	3920.1591

ts2c + 1 H_2O

Cartesian coordinates

C	0.772482	-0.501920	-0.015622
N	1.345164	0.733906	-0.019163
C	0.596230	1.855470	-0.010686
N	-0.711774	1.935174	0.001026
C	-1.321808	0.725578	0.004256
C	-0.635112	-0.484765	-0.004130
N	-2.674770	0.502688	0.016160
N	-1.602965	-1.457702	0.003161
C	-2.790247	-0.807789	0.015016
H	-3.725607	-1.347143	0.022542
H	-1.462765	-2.455126	-0.000061
H	1.158864	2.783469	-0.013836
O	1.501402	-1.548007	-0.025070
H	2.719923	0.468153	-0.022494
O	3.539493	-0.299851	-0.058607
H	4.030761	-0.295022	0.768677
H	2.732808	-1.089372	-0.026702

Vibrational frequencies

-1299.3995	79.5847	173.9228
224.2276	252.6189	305.1731
369.6951	512.1622	540.4936
555.3555	569.9288	584.0073
635.4494	643.8893	659.5510
689.7872	739.7738	755.1805
823.8441	923.1612	937.6061
969.3538	992.6690	1106.8524
1130.8733	1165.7518	1228.5761
1304.2128	1354.6212	1379.7594
1383.1419	1424.7170	1442.6720
1488.0918	1519.0667	1539.6903
1581.3501	1608.6680	1707.1951
1740.7715	2092.1491	3199.6338
3274.8199	3683.9278	3887.2341

1H-purin-6(7H)-one + 1 H_2O

Cartesian coordinates

C	0.737194	-0.564467	-0.027080

N	1.266579	0.724074	-0.031865
C	0.533101	1.873290	-0.017821
N	-0.759229	1.936743	0.001144
C	-1.367568	0.713009	0.006729
C	-0.685558	-0.494295	-0.006846
N	-2.716750	0.497234	0.026373
N	-1.653235	-1.463178	0.005149
C	-2.839733	-0.814228	0.024668
H	-3.776423	-1.350432	0.037202
H	-1.511198	-2.460837	-0.000023
H	1.116678	2.786660	-0.023270
O	1.449664	-1.565918	-0.041908
H	2.289902	0.770047	-0.042735
O	3.935562	-0.262684	-0.039595
H	4.280622	-0.270139	0.855740
H	3.292447	-0.990438	-0.058403

Vibrational frequencies

54.3275	125.8942	164.3634
184.1682	204.2792	287.3054
317.5496	337.9244	352.5378
528.1740	562.9176	563.3496
575.0638	633.0474	660.3521
680.2203	731.0692	733.9537
816.0598	887.6078	915.8220
919.4020	969.8481	982.1244
1114.9757	1141.7986	1184.0587
1246.9865	1320.6912	1372.4190
1428.5197	1439.9155	1493.4945
1511.1302	1578.0241	1594.7437
1652.3828	1671.5828	1766.0851
3216.9054	3278.7890	3411.4099
3678.7252	3688.0711	3926.0690

7H-purin-6-ol + 2 H_2O

Cartesian coordinates

C	0.255745	-0.468416	0.009782
N	0.861165	0.713770	-0.062107
C	0.106462	1.832902	-0.121312
N	-1.204805	1.929993	-0.116199
C	-1.827211	0.737734	-0.039618
C	-1.141714	-0.474708	0.025680
N	-3.181533	0.519349	-0.015174
N	-2.111913	-1.442738	0.089593
C	-3.297902	-0.787179	0.062174
H	-4.234218	-1.323583	0.102266
H	-1.978149	-2.439482	0.146234
H	0.669039	2.759791	-0.178864
O	0.920501	-1.597964	0.069465
H	2.652042	1.106697	0.074920
O	3.523867	-1.470205	-0.131159
H	3.794071	-1.676804	-1.028457

H	1.912724	-1.477422	-0.000548
O	3.624070	1.195399	0.174659
H	3.769889	-0.529565	0.005516
H	3.754418	1.477910	1.082184

Vibrational frequencies

30.7096	47.5642	94.3895
172.1468	174.3668	194.6792
223.5732	256.8164	287.6175
312.2054	367.4378	380.4940
403.3120	517.1799	537.1615
544.4646	569.6837	593.0485
650.5132	653.9933	723.8767
735.3611	753.4552	832.1474
915.3838	929.7205	965.6748
985.0764	990.8668	1024.4933
1119.2314	1153.2461	1207.8420
1289.5312	1332.3218	1378.8715
1412.1551	1436.9949	1446.6138
1476.8296	1549.0862	1558.2028
1622.7942	1659.9152	1666.1360
1716.1167	3054.9301	3191.6570
3274.3750	3434.3404	3509.1024
3686.4243	3924.4545	3926.1892

ts2c + 2 H_2O

Cartesian coordinates

C	-0.326560	-0.450014	-0.031670
N	-0.850784	0.806803	0.009171
C	-0.043946	1.889138	0.057554
N	1.267363	1.931251	0.070802
C	1.830475	0.698793	0.028019
C	1.090210	-0.473249	-0.022546
N	3.174453	0.415869	0.030102
N	2.013039	-1.489939	-0.051097
C	3.229941	-0.897867	-0.017936
H	4.139726	-1.479434	-0.030879
H	1.822836	-2.478087	-0.088075
H	-0.567893	2.840956	0.088734
O	-1.032886	-1.496927	-0.075407
H	-2.342658	1.038109	-0.040035
O	-3.495633	-1.333745	0.070651
H	-3.797586	-1.659977	0.922853
H	-2.448971	-1.453932	0.016163
O	-3.400852	1.044294	-0.054298
H	-3.591307	-0.162230	0.011077
H	-3.688405	1.396934	-0.900769

Vibrational frequencies

-810.6125	52.0268	60.8638
117.9757	171.6762	219.4074
240.3895	300.7005	309.3318

448.6884	458.9941	535.1232
545.3636	571.3124	586.5804
592.3694	624.0662	644.4594
663.6967	706.3568	739.2818
744.0491	754.7759	829.5619
919.8877	934.2255	970.7257
988.2447	1116.6557	1126.7581
1156.3551	1216.8958	1254.2364
1302.5212	1343.3213	1386.0950
1416.4266	1446.4289	1488.2067
1536.1883	1568.4446	1577.9737
1604.0825	1614.3390	1669.4861
1692.3469	1819.2904	2144.9344
2222.8978	3178.5729	3267.1188
3690.2592	3901.3671	3903.9808

1H-purin-6(7H)-one + 2 H_2O

Cartesian coordinates

C	-0.286243	-0.497653	-0.111165
N	-0.766550	0.801704	-0.037354
C	0.016450	1.911961	0.078186
N	1.310144	1.924264	0.133816
C	1.868918	0.680333	0.063144
C	1.136605	-0.490887	-0.055300
N	3.207072	0.404088	0.100531
N	2.061485	-1.500510	-0.089597
C	3.273502	-0.908013	0.006424
H	4.185877	-1.484853	0.002841
H	1.876501	-2.487860	-0.168781
H	-0.531277	2.846568	0.124440
O	-1.021480	-1.480731	-0.211181
H	-1.792291	0.944173	-0.080087
O	-3.731890	-1.463311	0.246329
H	-3.812600	-1.698739	1.172721
H	-2.779227	-1.551657	0.049474
O	-3.532222	1.214789	-0.128167
H	-3.792469	0.283760	0.031216
H	-3.810209	1.401349	-1.027180

Vibrational frequencies

25.8191	53.2654	73.9771
158.3103	176.5056	190.4480
211.4682	254.8047	284.7346
292.0553	340.7165	359.4881
379.5634	495.1711	534.8946
561.9005	566.8592	578.4286
631.8616	661.7800	694.5442
735.9197	740.3043	820.0962
914.9367	922.1036	927.7253
964.9724	970.2867	1021.3264
1117.4156	1144.5119	1194.3770
1250.8346	1321.5775	1373.9024

1430.0586	1442.3123	1496.5180
1535.5557	1585.2874	1600.7319
1655.7963	1662.9826	1681.5319
1755.9729	3183.2040	3216.2883
3274.0668	3505.0859	3585.1731
3682.3618	3927.2009	3930.2824

7H-purin-6-ol + 3 H_2O

Cartesian coordinates

C	-0.207774	-0.499099	-0.229053
N	0.423751	0.670888	-0.279885
C	-0.290491	1.807848	-0.128681
N	-1.584356	1.934977	0.065562
C	-2.234639	0.755834	0.111206
C	-1.591180	-0.472567	-0.031873
N	-3.580349	0.567464	0.301218
N	-2.577730	-1.419814	0.076606
C	-3.732174	-0.737394	0.271985
H	-4.673499	-1.253235	0.389508
H	-2.473062	-2.420164	0.022028
H	0.292776	2.722546	-0.176771
O	0.418608	-1.643556	-0.358844
H	2.162780	1.051319	-0.632394
O	3.014303	-1.558562	-0.541297
H	3.245641	-0.800430	-1.095834
H	1.414417	-1.540542	-0.439678
O	3.130047	1.184656	-0.749402
H	3.797804	0.635004	0.870323
H	3.244665	2.022147	-1.199913
O	3.970232	-0.040451	1.550779
H	3.365447	-1.274421	0.325580
H	4.925855	-0.081260	1.621246

Vibrational frequencies

26.8967	29.7907	69.5491
90.7673	151.8536	171.5610
178.0853	188.5612	223.9235
228.2478	256.6225	278.1784
313.3799	319.5498	370.8769
374.3380	442.1918	527.4454
540.2178	549.2075	571.8499
592.2074	613.8189	655.6373
663.8720	725.5465	733.6421
744.6752	818.5436	835.3457
880.6819	915.9506	937.9950
966.5102	990.4316	1080.4052
1120.4551	1153.3057	1207.3818
1291.3770	1331.2541	1380.6827
1412.5162	1436.1371	1446.9424
1477.6659	1550.5071	1559.9872
1623.0302	1654.8442	1680.5551
1710.7282	1719.2638	3008.3140

3189.0209	3273.2678	3418.0746
3570.3550	3642.8844	3687.5208
3793.8372	3932.6368	3948.3679

ts2c + 3 H_2O

Cartesian coordinates

C	0.149991	-0.457037	0.060578
N	-0.367711	0.802726	0.116467
C	0.447771	1.877052	0.096241
N	1.760120	1.922724	0.029499
C	2.316689	0.687372	-0.027319
C	1.570184	-0.479973	-0.015076
N	3.658887	0.397770	-0.103919
N	2.486172	-1.502143	-0.085808
C	3.705839	-0.916831	-0.136160
H	4.610762	-1.503173	-0.195981
H	2.288226	-2.489200	-0.097504
H	-0.069812	2.833190	0.141641
O	-0.548732	-1.502043	0.070119
H	-1.909971	1.287426	0.160058
O	-3.043826	-1.865183	0.347297
H	-3.212456	-1.916044	1.290942
H	-2.053119	-1.664348	0.238157
O	-2.841279	1.704554	0.149564
H	-3.741663	0.761840	-0.354405
H	-3.041144	1.943068	1.057588
O	-4.288661	-0.076911	-0.709915
H	-3.790320	-0.927860	-0.235561
H	-5.205644	-0.019276	-0.424708

Vibrational frequencies

-185.3084	22.6181	35.7192
61.7590	72.2421	108.7249
168.6525	212.5755	217.4565
261.5091	309.2456	381.5843
406.5839	413.2370	480.2075
488.9027	541.4396	556.7979
567.0213	583.4277	591.7361
661.8023	669.2827	684.4824
746.0081	747.2344	779.2301
832.9828	910.3354	924.5499
969.3390	976.8805	992.1541
1083.9451	1116.4317	1149.7465
1151.9896	1209.8619	1291.9935
1333.8501	1362.6333	1388.7362
1411.2042	1445.4512	1461.1179
1495.0131	1537.7157	1598.6911
1605.4857	1669.8073	1673.5365
1682.3891	1784.9159	1833.0840
2140.5662	2705.2919	2802.3301
3163.0718	3267.2614	3691.8455
3892.4326	3917.6035	3920.0395

1H-purin-6(7H)-one + 3 H_2O

Cartesian coordinates

C	-0.212951	-0.556573	-0.140962
N	0.302280	0.727589	-0.205143
C	-0.443126	1.866801	-0.134159
N	-1.730008	1.924825	-0.001263
C	-2.322705	0.696581	0.069028
C	-1.628573	-0.501981	0.004836
N	-3.662114	0.464450	0.212052
N	-2.578424	-1.482822	0.112407
C	-3.766925	-0.848384	0.232920
H	-4.691778	-1.395572	0.334654
H	-2.423687	-2.478496	0.103029
H	0.135810	2.781298	-0.198252
O	0.488194	-1.567178	-0.203640
H	1.323713	0.865192	-0.306882
O	3.196925	-1.811237	-0.491754
H	3.374301	-1.528956	-1.390852
H	2.229890	-1.716502	-0.386739
O	2.889359	1.644649	-0.394832
H	3.501278	1.162065	0.200909
H	3.282866	1.576664	-1.266613
O	4.402091	-0.004099	1.133727
H	4.039523	-0.753362	0.615806
H	5.339076	0.013634	0.930577

Vibrational frequencies

21.1621	31.9238	46.5302
67.7348	78.0675	157.1587
168.9243	190.2438	214.8636
261.1778	268.7938	277.9158
294.0843	318.4985	342.6389
382.4648	385.9574	494.4938
501.8053	537.6839	563.4884
566.6514	580.5263	634.6091
662.3084	727.2124	734.2601
742.3068	786.7467	821.7260
916.1284	918.4265	940.9831
969.6164	974.1769	1053.4568
1117.5103	1144.7639	1189.8186
1245.7163	1322.6812	1366.9242
1424.8269	1440.4734	1493.2291
1523.4996	1581.7605	1596.7250
1660.2676	1667.6888	1677.0458
1680.5513	1750.4333	3201.6028
3217.2640	3278.7528	3453.0494
3520.8165	3575.1221	3680.0935
3931.9651	3934.9454	3936.8675

SCRF/PCM//ωB97X-D/6-311G(d,p) for *2-amino-7H-purin-6-ol → ts2j → guanine* pathway with H_2O solvent molecules

2-amino-7H-purin-6-ol + 0 H_2O

Cartesian coordinates

C	-0.295305	1.295326	-0.001556
N	-1.519081	0.813292	-0.004066
C	-1.680685	-0.534724	-0.006924
N	-0.724517	-1.456670	-0.001012
C	0.516585	-0.946261	-0.001630
C	0.788848	0.422748	-0.004203
N	1.692061	-1.658079	0.003630
N	2.162434	0.529716	0.000064
C	2.632623	-0.737724	0.004410
H	3.693572	-0.939698	0.007639
H	2.711460	1.373343	-0.000527
N	-2.976835	-0.964064	-0.059054
H	-3.679555	-0.301192	0.222816
H	-3.137166	-1.922515	0.202945
O	-0.103528	2.613540	0.005436
H	-0.970913	3.036176	0.006107

Vibrational frequencies

137.3864	176.7404	244.0107
298.7586	344.1435	366.9902
421.8509	459.3516	496.0990
507.9714	509.9027	564.2620
642.5828	648.7923	672.1938
711.2118	764.7629	821.8698
846.0132	915.8808	961.6057
1045.4502	1100.9431	1147.8736
1178.0760	1234.0364	1278.1102
1363.1240	1376.7117	1424.6863
1469.3150	1492.6800	1539.5566
1554.8040	1636.8536	1641.3635
1723.6679	3270.7520	3628.1309
3695.3637	3747.5881	3832.4456

ts2j + 0 H_2O

Cartesian coordinates

C	-0.279219	1.332050	-0.000408
N	-1.489443	0.727534	-0.002541
C	-1.644469	-0.617922	-0.004736
N	-0.623141	-1.462431	-0.000463
C	0.593348	-0.882589	-0.000930
C	0.833178	0.500480	-0.002028
N	1.788142	-1.555124	0.002337
N	2.203615	0.641977	0.000886
C	2.705753	-0.609294	0.003050
H	3.771282	-0.784848	0.005026
H	2.729350	1.500570	0.000729
O	-0.516356	2.591278	0.003097
H	-1.716866	2.014345	0.000668
N	-2.909726	-1.100214	-0.052178

H	-3.026971	-2.075781	0.164246
H	-3.663630	-0.483052	0.198581

Vibrational frequencies

-1948.1756	145.7479	151.7621
222.7146	328.7342	355.5825
360.8918	375.6440	457.5806
499.0564	505.4116	583.5402
621.2218	667.7690	674.1039
742.5388	746.4972	801.1224
851.5748	918.6546	961.6330
1073.1416	1092.6981	1139.5990
1152.3555	1199.5371	1286.3794
1339.0057	1392.1417	1406.8774
1487.7549	1496.6672	1540.2926
1565.8106	1611.4667	1645.2950
1727.1553	2143.7391	3273.6714
3631.4540	3694.2637	3752.1074

guanine + 0 H_2O

Cartesian coordinates

C	-0.194352	1.434726	0.001204
N	-1.455472	0.819649	-0.001070
C	-1.687245	-0.536867	-0.001824
N	-0.741314	-1.435307	0.004538
C	0.519320	-0.918469	0.000692
C	0.817899	0.433982	0.001581
O	-0.080533	2.649595	0.000174
H	-2.240011	1.456655	-0.024935
N	1.671996	-1.656233	0.000497
N	2.190694	0.512393	0.001494
C	2.639826	-0.759044	0.000863
H	3.695344	-0.985533	0.000341
H	2.748566	1.350821	0.001492
N	-2.990758	-0.920281	-0.061383
H	-3.153836	-1.895387	0.130361
H	-3.704500	-0.290837	0.267718

Vibrational frequencies

143.7244	160.6886	195.6856
308.7912	338.5809	350.1567
372.6671	462.0645	495.9042
534.3974	548.6756	604.7389
643.7657	658.6664	681.3269
736.0099	748.9592	807.2155
846.8258	900.2366	968.1245
1054.4510	1113.7919	1141.7958
1173.3194	1216.0289	1304.9579
1360.8535	1398.2039	1429.5279
1492.4800	1518.4396	1586.4201
1610.0721	1638.9423	1672.8581
1785.4330	3272.2638	3622.6539

3630.0959 3688.8925 3736.1875

2-amino-7H-purin-6-ol + 1 H_2O

Cartesian coordinates

C	0.491255	-0.789797	-0.029325
N	1.255401	0.293126	-0.027850
C	0.660128	1.514021	-0.004736
N	-0.641788	1.769405	0.011892
C	-1.407199	0.665865	0.012958
C	-0.892733	-0.629931	-0.006324
N	-2.780426	0.626161	0.029261
N	-1.988051	-1.465756	-0.001465
C	-3.070950	-0.657733	0.020365
H	-4.071254	-1.064809	0.029226
H	-1.990216	-2.472399	-0.011439
O	1.030968	-1.996253	-0.056077
H	3.145926	-0.389785	-0.022140
O	3.606822	-1.247073	-0.029258
H	4.003713	-1.324996	0.841503
H	2.015883	-1.907804	-0.051483
N	1.516317	2.577875	0.045102
H	2.459941	2.414515	-0.264056
H	1.120517	3.471648	-0.195138

Vibrational frequencies

52.2258	107.3818	139.4296
183.7409	186.5945	237.4896
316.4297	334.4598	364.7711
370.0840	390.3467	411.4833
446.8670	509.8693	510.2984
570.9033	639.9003	647.2777
682.4081	714.4945	718.4237
763.7415	821.3329	849.3667
891.8697	917.3298	962.2583
1070.7126	1104.7261	1146.5585
1181.5467	1256.9726	1315.5274
1380.3235	1414.6812	1443.0765
1475.1467	1512.8792	1538.0738
1556.2503	1634.4526	1639.7372
1646.7172	1726.8990	3273.4155
3319.4731	3627.1868	3650.7017
3695.1988	3745.5638	3922.1128

ts2j + 1 H_2O

Cartesian coordinates

C	0.467332	-0.902482	-0.022153
N	1.289751	0.181731	-0.019819
C	0.795099	1.447286	-0.003138
N	-0.481947	1.782744	0.007801
C	-1.320566	0.725114	0.009260
C	-0.904000	-0.602112	-0.005500
N	-2.691278	0.787934	0.021363

N	-2.057873	-1.354913	-0.001921
C	-3.078616	-0.471975	0.014307
H	-4.106903	-0.801825	0.020764
H	-2.129488	-2.359035	-0.009638
O	0.968230	-2.077191	-0.039912
H	2.551191	-0.357421	-0.011233
O	3.216275	-1.283464	-0.042824
H	3.677193	-1.382222	0.795486
H	2.248372	-1.887139	-0.028037
N	1.725830	2.445644	0.049551
H	2.653250	2.232239	-0.278547
H	1.383465	3.363693	-0.182378

Vibrational frequencies

-1423.7114	72.4334	142.1444
186.4982	226.6256	237.3306
316.8857	372.0928	389.8015
397.7533	454.6979	496.1553
512.9532	546.0421	582.9384
618.9670	635.6202	653.5891
656.9122	732.1577	736.5536
757.5091	816.1319	857.4934
913.2392	964.8881	1026.1019
1111.2947	1135.2149	1148.2358
1193.1949	1252.5819	1311.2341
1380.4159	1396.8158	1429.2940
1482.8273	1503.6324	1513.8796
1542.4822	1571.8835	1620.3837
1645.8144	1699.1317	1725.1469
2065.3884	3268.4014	3623.7107
3693.7860	3739.1699	3888.7992

guanine + 1 H_2O

Cartesian coordinates

C	0.457710	-0.939894	-0.041304
N	1.206909	0.236753	-0.037268
C	0.684965	1.506843	-0.012332
N	-0.593999	1.772019	0.010627
C	-1.390205	0.669335	0.015369
C	-0.927962	-0.637887	-0.013627
N	-2.758190	0.685184	0.041885
N	-2.051883	-1.430396	-0.003742
C	-3.104460	-0.588008	0.029339
H	-4.120048	-0.953966	0.043602
H	-2.084023	-2.436856	-0.018556
O	0.999314	-2.045087	-0.065867
H	2.220372	0.089267	-0.026047
O	3.663280	-1.201710	-0.009196
H	3.983393	-1.276323	0.892278
H	2.897017	-1.798894	-0.046050
N	1.590590	2.520444	0.037985
H	2.518334	2.364048	-0.321389

H	1.209927	3.436735	-0.134417

Vibrational frequencies

52.4329	114.7820	143.7208
167.3379	183.2872	200.5495
310.6112	328.2178	332.1183
348.1949	363.0560	375.0226
470.8072	500.1109	536.4641
554.2326	644.1478	654.4843
691.8765	708.9207	730.5640
741.0890	807.4840	845.2284
847.6626	906.7629	966.5940
1069.6413	1119.0105	1143.7428
1182.6216	1226.4315	1307.8037
1395.5916	1406.5618	1437.2433
1498.7679	1521.7945	1587.5819
1610.7457	1642.4002	1652.5765
1677.7253	1762.8986	3274.8128
3403.0016	3622.1291	3667.2878
3691.4154	3735.3818	3926.3738

2-amino-7H-purin-6-ol + 2 H_2O

Cartesian coordinates

C	0.121530	-0.739974	0.042778
N	0.824872	0.383787	-0.001455
C	0.167881	1.575059	-0.063989
N	-1.143369	1.763576	-0.084144
C	-1.851172	0.622596	-0.024905
C	-1.270333	-0.642136	0.042595
N	-3.219965	0.512486	-0.030642
N	-2.320956	-1.532941	0.075080
C	-3.444164	-0.783614	0.031068
H	-4.422343	-1.240902	0.047669
H	-2.270783	-2.537187	0.125090
O	0.702470	-1.918231	0.090286
H	2.604148	0.579256	0.210848
O	3.321004	-1.969490	-0.209455
H	3.526539	-2.152148	-1.128873
H	1.695266	-1.864969	0.000069
O	3.581233	0.689001	0.234036
H	3.650534	-1.062324	-0.045594
H	3.787737	0.926395	1.140477
N	0.970993	2.680531	-0.065610
H	1.932654	2.555518	-0.338929
H	0.535110	3.542458	-0.347576

Vibrational frequencies

39.9306	47.2041	95.5533
141.4776	184.7992	186.4513
198.2234	239.0533	252.8036
282.6034	347.7961	361.1743
371.0401	388.1360	389.5030

421.0924	461.5660	504.9945
510.7555	515.0053	577.3899
647.0582	649.5516	704.4564
717.6927	764.4263	777.6186
822.2767	852.9177	917.0820
965.2039	984.1335	1049.7913
1075.0177	1114.4088	1152.2811
1187.2269	1265.0547	1317.6720
1382.9805	1410.3476	1436.3592
1484.2611	1502.1970	1547.8113
1559.9921	1634.8560	1648.3613
1651.0032	1662.0055	1720.4594
3140.3222	3275.6578	3402.9008
3542.9322	3617.6329	3694.5845
3738.3395	3924.8615	3926.9352

ts2j + 2 H_2O

Cartesian coordinates

C	-0.215131	-0.727340	-0.027109
N	-0.828572	0.486048	0.001008
C	-0.101901	1.635368	0.048705
N	1.212597	1.752736	0.062977
C	1.851301	0.561508	0.015788
C	1.198205	-0.660140	-0.027383
N	3.212043	0.373337	0.014419
N	2.193293	-1.612626	-0.053961
C	3.361517	-0.935833	-0.028842
H	4.311205	-1.449645	-0.044283
H	2.075391	-2.611740	-0.088926
O	-0.853983	-1.818877	-0.054817
H	-2.291516	0.582853	-0.146048
O	-3.311123	-1.819316	0.156646
H	-3.569943	-2.076648	1.045704
H	-2.255430	-1.869466	0.082195
O	-3.361740	0.535500	-0.198797
H	-3.484491	-0.669224	-0.014710
H	-3.635023	0.782215	-1.086460
N	-0.844346	2.792595	0.035124
H	-1.778711	2.731821	0.407813
H	-0.335774	3.615359	0.316538

Vibrational frequencies

-904.5860	43.3868	52.4083
108.9782	142.6962	180.9809
228.3298	240.6169	299.2502
356.8824	374.2443	416.0668
449.5476	459.6906	515.8428
518.7940	534.5670	548.0253
590.3603	618.4187	644.8586
657.2161	671.5456	738.7038
739.8866	749.9028	766.1422
820.5404	863.9158	904.4693

968.4695	1080.4483	1120.8964
1142.4105	1176.0592	1195.7141
1254.2898	1314.9640	1321.5372
1385.5179	1431.3492	1458.1473
1498.9215	1533.7913	1562.4818
1572.4785	1612.0644	1622.0444
1646.2491	1667.1621	1681.1546
1794.6747	1970.0168	2163.9804
3271.8066	3615.0747	3691.4424
3726.6376	3899.8888	3901.4713

guanine + 2 H_2O

Cartesian coordinates

C	-0.086266	-0.867669	-0.197958
N	-0.772096	0.336412	-0.156709
C	-0.198112	1.573424	0.012082
N	1.088061	1.776900	0.130865
C	1.830241	0.638539	0.070004
C	1.308958	-0.638248	-0.089352
N	3.194248	0.580110	0.170366
N	2.392014	-1.486198	-0.080197
C	3.479629	-0.704654	0.074086
H	4.474095	-1.123145	0.111777
H	2.378033	-2.488818	-0.173749
O	-0.673595	-1.946449	-0.314337
H	-1.795020	0.316058	-0.243275
O	-3.344141	-1.953758	0.409895
H	-3.304420	-2.145768	1.348859
H	-2.422449	-2.049457	0.098773
O	-3.573160	0.693261	-0.155350
H	-3.694286	-0.243013	0.108496
H	-3.951095	0.758343	-1.034791
N	-1.073195	2.609752	0.012263
H	-2.049727	2.410959	0.176592
H	-0.717894	3.493229	0.336363

Vibrational frequencies

36.7307	58.2312	61.1492
147.4099	158.7113	178.4128
188.9529	206.0278	254.7314
283.8748	335.4193	352.5568
362.8853	373.9981	397.4009
413.5714	486.7575	505.0346
518.2315	529.4630	558.2954
650.4611	654.9721	696.3642
725.3036	740.1609	748.3207
809.1738	846.2309	869.8755
906.5635	940.4884	967.5458
1079.1880	1129.0090	1151.7486
1185.3026	1237.6293	1314.4226
1392.4777	1405.0639	1437.6117
1497.4177	1525.1824	1597.0257

1609.7929	1644.4901	1656.5914
1669.0490	1689.2077	1748.1996
3276.1521	3336.3446	3504.2317
3576.4855	3597.3469	3689.5538
3734.2891	3928.6369	3930.5482

2-amino-7H-purin-6-ol + 3 H_2O

Cartesian coordinates

C	-0.284359	-0.745868	-0.180341
N	0.424495	0.376089	-0.208491
C	-0.217227	1.566920	-0.053981
N	-1.516961	1.760479	0.107244
C	-2.233476	0.622888	0.109235
C	-1.667694	-0.642588	-0.027558
N	-3.594220	0.517513	0.258598
N	-2.719001	-1.529879	0.045786
C	-3.828617	-0.777471	0.212820
H	-4.804598	-1.231678	0.298625
H	-2.677987	-2.534000	-0.014262
O	0.282757	-1.924772	-0.294262
H	2.121675	0.596960	-0.804071
O	2.899062	-1.962211	-0.326039
H	3.173986	-1.315806	-0.990289
H	1.282833	-1.872227	-0.312382
O	3.081810	0.732462	-0.970371
H	3.779246	0.422888	0.732330
H	3.158469	1.394446	-1.658866
O	3.892901	-0.152660	1.507117
H	3.236830	-1.548997	0.492327
H	4.842137	-0.232144	1.619189
N	0.589070	2.671900	-0.116303
H	0.178472	3.525048	0.225950
H	1.561263	2.536958	0.110999

Vibrational frequencies

27.3789	36.1376	66.0653
89.7325	142.9167	154.8918
174.6549	183.4017	191.8248
215.7156	246.3778	264.0059
275.7220	310.5669	347.9726
351.3209	373.4121	383.5829
414.5554	475.5272	490.9076
507.9783	511.8953	518.7669
575.7807	595.5484	647.1448
651.5954	701.6177	711.9433
722.0622	767.1453	825.6918
834.1588	853.7877	922.8013
930.1939	964.7143	1069.4697
1072.1791	1112.6108	1148.6171
1185.4839	1264.3564	1316.2550
1383.0732	1406.2774	1434.9656
1482.9826	1495.1364	1546.2869

1559.6513	1633.1564	1640.8378
1651.7798	1670.7149	1711.1279
1720.6494	3063.3101	3267.3443
3405.0865	3587.4308	3617.6556
3686.5998	3694.4552	3733.9322
3805.5173	3933.7615	3945.1649

ts2j + 3 H_2O

Cartesian coordinates

C	-0.166605	-0.660906	-0.118976
N	0.341904	0.601861	-0.139965
C	-0.480241	1.682020	-0.053265
N	-1.798116	1.693186	0.058510
C	-2.334558	0.450800	0.072116
C	-1.583514	-0.707983	-0.013840
N	-3.671952	0.145961	0.176138
N	-2.491475	-1.743757	0.040075
C	-3.709773	-1.171825	0.151593
H	-4.609770	-1.765816	0.211609
H	-2.286856	-2.728483	0.003373
O	0.545823	-1.693955	-0.182692
H	1.852595	0.966537	-0.243736
O	3.053609	-2.152412	-0.265853
H	3.286849	-2.244974	-1.192244
H	2.070785	-1.916262	-0.239769
O	2.813666	1.364619	-0.249193
H	3.682418	0.504325	0.354256
H	3.043620	1.531444	-1.166527
O	4.237966	-0.304792	0.800068
H	3.794868	-1.171455	0.348578
H	5.168801	-0.244388	0.564092
N	0.149509	2.903818	-0.135563
H	-0.398003	3.678330	0.202345
H	1.125235	2.922945	0.119246

Vibrational frequencies

-180.4060	28.4703	31.3553
69.3958	88.0270	123.1165
143.0002	178.4382	214.2701
231.2918	276.4324	358.0940
372.1112	394.0181	404.7967
410.3625	462.5336	482.9304
490.5545	510.7640	522.0065
530.0212	569.1075	581.7184
658.2148	666.0385	690.0783
726.8379	741.1158	766.7399
779.6494	822.0429	856.1993
902.3344	966.1416	970.6308
1057.9126	1080.9423	1120.2272
1148.1532	1179.8013	1223.9236
1272.1470	1311.6451	1377.8391
1424.1527	1433.0146	1445.2538

1471.2499	1503.7882	1547.5294
1597.1457	1622.0225	1648.9563
1662.8563	1674.9166	1677.4282
1784.8103	1846.2380	2091.7860
2382.5429	2920.9804	3264.9970
3608.1800	3696.1282	3725.3745
3890.9412	3913.4799	3920.1893

guanine + 3 H_2O

Cartesian coordinates

C	-0.302098	-0.829286	-0.222055
N	0.313003	0.412772	-0.259487
C	-0.334061	1.621342	-0.107841
N	-1.624157	1.743035	0.085355
C	-2.291175	0.560629	0.120515
C	-1.697956	-0.684918	-0.025421
N	-3.640237	0.419628	0.308880
N	-2.720421	-1.600175	0.080308
C	-3.845372	-0.883607	0.276480
H	-4.806308	-1.361712	0.392871
H	-2.645789	-2.602817	0.022984
O	0.333215	-1.879702	-0.347547
H	1.329725	0.450139	-0.390840
O	3.046754	-2.118482	-0.438898
H	3.283811	-1.842226	-1.326014
H	2.071577	-2.043790	-0.405365
O	2.976073	1.356565	-0.398718
H	3.518386	0.851939	0.247644
H	3.447953	1.314212	-1.232062
O	4.220044	-0.353653	1.254893
H	3.850320	-1.089521	0.722522
H	5.171659	-0.421833	1.158581
N	0.455351	2.712371	-0.198938
H	0.047342	3.592610	0.062923
H	1.461831	2.596804	-0.173980

Vibrational frequencies

25.8271	37.9498	58.2323
69.3356	101.3344	144.7201
159.2446	171.3776	184.8194
208.2885	266.7438	275.1029
289.1103	315.6685	337.8858
342.9565	346.8537	369.5034
375.2541	397.8168	498.5556
503.3842	506.1736	530.4420
555.8429	625.2257	655.1281
657.0450	698.5072	728.4178
740.5447	748.5676	799.9306
810.8354	846.9207	896.2143
922.0864	968.0578	987.6749
1067.4299	1130.1622	1154.5829
1185.5491	1237.7949	1315.5772

1386.6709	1401.8208	1435.7925
1493.	1522.2857	1598.6249
1609.1958	1635.6643	1659.4459
1670.2468	1677.1328	1682.1523
1746.9883	3268.3936	3363.3173
3423.5395	3493.7222	3538.4550
3554.0594	3690.5246	3731.4766
3933.0289	3934.7709	3938.9220

III. Optimized coordinates (Å) and vibrational frequencies (cm^{-1}) in uracil and citosine pathways

1) ωB97X-D/6-311G(d,p) without SCRF/PCM

Reactants

pyrimidine

Cartesian coordinates

C	-0.978124	0.579272	0.001708
C	-0.950589	-0.807378	0.000614
N	0.188547	-1.496918	-0.001441
C	1.304824	-0.772295	-0.002298
N	1.403288	0.554082	-0.001458
C	0.250821	1.221785	0.000578
H	-1.909236	1.130982	0.003522
H	-1.867931	-1.389254	0.001329
H	2.238996	-1.326180	-0.003835
H	0.319406	2.305904	0.001280

Vibrational frequencies

353.5751	409.8202	638.0161
702.5823	739.2454	828.8752
990.9826	1009.5607	1026.2975
1035.9673	1092.5513	1101.8876
1178.3549	1221.0585	1271.6789
1396.3478	1458.9340	1506.3242
1650.1573	1652.5124	3184.2959
3187.4920	3196.2353	3234.5808

hydroxyl radical

Cartesian coordinates

O	0.325555	0.356863	0.000000
H	-0.644419	0.356863	0.000000

Vibrational frequencies

3793.3852

amino radical

Cartesian coordinates

N	-0.535941	-0.013571	0.000000
H	-0.906803	0.945100	0.000000
H	0.479723	0.144589	0.000000

Vibrational frequencies

1530.0306	3393.5435	3484.3297

Intermediates

i8

Cartesian coordinates

C	-1.329995	0.771642	0.204065
C	-1.372305	-0.640376	0.060309
N	-0.315653	-1.376659	-0.059273

C	0.955991	-0.710252	0.075024
N	1.041986	0.734264	-0.023584
C	-0.062279	1.398360	0.085667
O	1.827421	-1.280812	-0.852849
H	-2.236221	1.354225	0.304081
H	-2.334569	-1.146963	0.008577
H	1.282104	-0.940183	1.111217
H	0.002840	2.484437	0.047682
H	2.540680	-0.647683	-0.960915

Vibrational frequencies

91.0964	289.1598	335.9637
433.1089	482.9139	545.6179
606.0703	694.9722	760.3592
896.4924	977.6950	989.5233
1005.3715	1007.0544	1017.2384
1096.0687	1190.0884	1255.5734
1315.9142	1331.6985	1382.4580
1420.4446	1431.2162	1538.8409
1596.5782	2881.9187	3148.6415
3155.9941	3234.2351	3899.4164

pyrimidin-2-ol

Cartesian coordinates

C	-1.257448	0.710900	0.110756
C	-1.267542	-0.677958	0.103931
N	-0.163872	-1.410220	0.006095
C	0.967046	-0.720659	-0.086034
N	1.111007	0.603408	-0.090947
C	-0.011966	1.309178	0.008274
O	2.081502	-1.445605	-0.184602
H	-2.166467	1.290553	0.191249
H	-2.199129	-1.231961	0.179981
H	0.098829	2.389622	0.004757
H	2.808042	-0.817257	-0.243463

Vibrational frequencies

191.0893	420.3169	463.7934
532.5413	586.7855	608.3825
657.1636	812.2981	840.7802
908.0079	1008.3534	1015.8457
1020.7902	1109.2234	1113.5936
1222.4603	1273.0001	1381.0210
1398.5228	1498.2474	1522.1487
1657.9010	1677.1302	3184.3877
3190.2976	3244.6321	3871.2564

pyrimidin-2(1H)-one

Cartesian coordinates

C	-1.061205	0.785915	0.002443
C	-1.033912	-0.569229	0.000584
N	0.158255	-1.203287	-0.001703

C	1.410742	-0.545707	-0.002495
N	1.360461	0.840279	-0.000585
C	0.206196	1.434385	0.001675
O	2.421142	-1.202327	-0.004760
H	-1.987248	1.340450	0.004577
H	-1.919457	-1.193085	0.000683
H	0.210092	-2.210857	-0.003354
H	0.234935	2.523462	0.002938

Vibrational frequencies

126.7953	396.5920	489.8854
499.6386	580.2783	636.8469
722.5145	770.8089	822.8613
851.1074	981.8535	1008.4450
1010.9633	1035.0375	1128.4276
1166.0728	1237.9485	1397.8420
1456.6883	1509.9173	1609.2137
1717.4712	1851.5652	3151.1835
3226.7473	3262.8891	3652.9377

i9

Cartesian coordinates

C	1.235287	-0.471273	-0.028926
C	-1.047655	1.180166	0.113942
C	0.151999	1.707792	-0.075236
H	-1.946423	1.772233	0.156634
H	0.323825	2.764973	-0.209708
C	-1.150860	-0.304910	0.326196
H	-1.131153	-0.495835	1.423351
N	-0.038193	-1.029234	-0.189248
N	1.285907	0.905006	-0.101668
H	2.204557	1.309780	-0.134117
O	2.221782	-1.155282	0.097304
O	-2.352737	-0.773320	-0.209703
H	-2.269787	-1.723389	-0.316417

Vibrational frequencies

94.6667	118.6712	217.9213
339.7563	361.2392	457.6403
474.8623	547.9471	551.5432
637.5359	725.3845	741.9999
803.7368	908.3685	958.6148
971.4368	1068.7227	1111.5002
1178.8724	1180.9219	1212.3536
1282.2980	1325.1702	1389.6379
1423.8048	1480.9642	1746.6527
1784.1296	2815.2279	3232.1865
3262.9575	3682.2165	3881.4750

4-hydroxypyrimidin-2(*1H*)-one

Cartesian coordinates

C	-0.004275	-1.709358	0.000000

C	-1.214064	0.402280	0.000000
C	1.098068	0.356088	0.000000
C	1.181507	-1.066107	0.000000
H	-0.091513	-2.786304	0.000000
H	2.127194	-1.579101	0.000000
O	-2.290604	0.946600	0.000000
N	-1.155255	-1.007625	0.000000
H	-2.047895	-1.471146	0.000000
N	0.000000	1.045132	0.000000
O	2.253367	1.018380	0.000000
H	2.029480	1.956742	0.000000

Vibrational frequencies

142.9226	216.7469	381.4758
421.0230	541.4117	559.2685
581.5143	607.4049	662.0499
753.2647	786.8686	806.7425
817.0073	964.0410	999.5229
1019.2862	1126.5651	1209.3966
1234.2427	1287.9302	1376.3235
1483.3041	1529.7131	1631.0134
1722.1631	1833.4078	3227.1221
3273.1260	3665.3234	3813.3346

i10

Cartesian coordinates

C	-1.149960	0.225754	-0.160221
C	-1.145025	-1.102155	-0.132313
N	0.053473	-1.810453	-0.125052
C	1.288208	-1.189869	-0.064632
N	1.261681	0.163418	0.293809
C	0.162693	0.973824	-0.190950
O	2.325339	-1.782468	-0.245262
N	0.047746	2.237778	0.499885
H	-2.064138	0.800207	-0.192999
H	-2.044855	-1.703005	-0.126010
H	0.066131	-2.810534	-0.236995
H	0.399649	1.201093	-1.249010
H	0.929784	2.734579	0.446505
H	-0.130726	2.061831	1.483249

Vibrational frequencies

72.4318	111.0002	278.1215
336.5937	355.7393	452.2301
464.6137	540.5867	549.6514
611.2084	721.6347	745.5348
795.8501	881.0440	914.0237
962.5342	975.1478	1056.2537
1118.1081	1145.4883	1189.7753
1220.3971	1269.5464	1293.3341
1381.8801	1420.2060	1485.3395
1674.7346	1747.9934	1792.0796

2918.8218	3229.9642	3256.2129
3532.6261	3615.9857	3682.9208

Transition states

ts3a

Cartesian coordinates

C	-1.340088	0.015843	-0.146653
C	-0.599754	1.183086	-0.011588
N	0.708209	1.171436	0.204010
C	1.299347	-0.053425	0.216591
N	0.649470	-1.246410	0.201688
C	-0.648057	-1.192091	-0.008029
H	-2.407986	0.039005	-0.320720
H	-1.075590	2.158477	-0.059616
H	2.315690	-0.081627	0.589445
H	-1.175427	-2.141550	-0.050647
O	1.896635	0.037538	-1.626004
H	2.028954	0.995514	-1.665442

Vibrational frequencies

-552.9455	131.9348	202.9861
295.4802	367.1505	420.4354
628.9460	680.0294	734.3122
815.7042	838.3139	940.4137
1001.1912	1009.3133	1026.0047
1075.3886	1104.2245	1134.8743
1222.1369	1259.3146	1383.5048
1416.6879	1496.3296	1579.9537
1611.3117	3170.5018	3183.4951
3219.7882	3227.4661	3811.9368

ts3b

Cartesian coordinates

C	-1.770435	0.048475	-0.010248
C	-1.077848	-1.159396	-0.050337
N	0.242552	-1.236582	-0.065980
C	0.884509	-0.050559	0.033645
N	0.322673	1.179612	-0.080982
C	-1.000752	1.205182	-0.062619
O	2.211876	-0.110903	-0.153506
H	-2.851054	0.084898	-0.003450
H	-1.609787	-2.105670	-0.096699
H	0.828328	-0.048717	1.706453
H	-1.463463	2.186371	-0.118016
H	2.522985	0.799233	-0.167164

Vibrational frequencies

-1216.3752	184.1409	400.9495
445.9960	516.1255	543.8510
566.5052	584.5707	653.2054
674.6354	798.9377	830.5452
917.4248	1007.0461	1011.2981

1015.0416	1096.7977	1102.0419
1198.5357	1267.1985	1373.9670
1387.5376	1462.8375	1500.3846
1600.4503	1647.9433	3181.7969
3185.2365	3243.5651	3876.3025

ts3c

Cartesian coordinates

C	1.755523	0.034104	-0.007141
C	1.056045	-1.158146	0.054276
N	-0.267709	-1.101369	0.095630
C	-0.928327	0.100288	0.078312
N	-0.320702	1.289039	0.020183
C	1.004058	1.216503	-0.020756
O	-2.159570	-0.198821	0.128504
H	2.834675	0.054513	-0.043016
H	1.529102	-2.133206	0.070481
H	1.519957	2.172511	-0.068376
H	-1.501910	-1.392220	0.145602

Vibrational frequencies

-1898.2116	159.6504	408.8017
497.1624	563.7865	612.5960
709.3703	784.0842	797.9717
931.9785	996.3586	1026.7525
1028.4544	1080.8532	1128.2307
1143.2964	1240.9308	1308.7944
1411.6324	1493.3626	1587.6913
1635.5295	1725.4774	2182.5498
3169.3353	3217.7898	3254.3364

ts3d

Cartesian coordinates

C	-1.155400	-0.250681	-0.113936
C	1.340981	1.028816	-0.275394
C	0.276943	1.687960	0.206602
H	2.314662	1.481937	-0.345213
H	0.308689	2.716366	0.536097
C	1.124838	-0.336419	-0.667806
H	1.890551	-0.830230	-1.251654
N	-0.084463	-0.903663	-0.718205
N	-0.927044	1.063825	0.295609
H	-1.729354	1.540017	0.670929
O	-2.242460	-0.754629	0.026289
O	1.453166	-1.322779	0.941456
H	1.086186	-2.188021	0.709258

Vibrational frequencies

-506.3900	107.8177	128.4065
234.2123	346.7432	411.1604
498.1158	515.9144	577.0564
628.2629	664.6951	765.4258

791.3191 843.8368 849.3475
991.7122 994.1620 1009.9589
1063.0147 1126.9203 1195.3290
1251.5892 1359.7687 1435.0280
1469.6759 1553.4852 1703.0303
1809.8396 3192.5007 3226.4274
3267.4003 3664.6202 3790.3483

ts3e

Cartesian coordinates

C 1.195396 -0.509084 -0.006405
C -1.063958 1.181178 -0.018563
C 0.173188 1.711709 -0.052251
H -1.964782 1.769188 -0.026564
H 0.358515 2.774322 -0.107419
C -1.115102 -0.261353 0.066379
H -1.118055 -0.100275 1.696391
N -0.063488 -1.051437 -0.038718
N 1.256242 0.903850 -0.008368
H 2.186834 1.284440 -0.039590
O 2.224917 -1.138102 -0.003959
O -2.321649 -0.819184 -0.117051
H -2.175081 -1.770968 -0.160098

Vibrational frequencies

-1181.4534 136.9319 197.3877
308.7703 378.3474 438.1005
506.4981 544.3637 563.1207
575.6020 645.5269 663.4781
739.2599 773.2905 797.0489
839.0575 956.5929 983.8494
1002.1141 1121.2470 1194.3214
1217.1081 1265.8985 1362.2867
1473.7802 1482.9072 1578.5928
1689.7879 1826.9889 3230.1446
3276.0576 3664.6679 3823.1652

ts3f

Cartesian coordinates

C -0.099306 -1.715152 0.000000
C 1.212731 0.356555 0.000000
C -1.185589 0.346705 0.000000
C -1.288444 -1.068865 0.000000
H -0.030955 -2.793914 0.000000
H -2.233686 -1.581557 0.000000
O 2.300982 0.869677 0.000000
N 1.078976 -1.052879 0.000000
H 1.949973 -1.555808 0.000000
N 0.000000 0.979178 0.000000
O -2.069792 1.258105 0.000000
H -0.924035 1.909477 0.000000

Vibrational frequencies

-1924.8422 166.5549 180.4213
413.2563 413.3807 534.1341
599.5320 622.6723 649.9211
723.6433 786.8057 787.9727
801.8481 1007.6288 1008.1330
1063.2937 1111.8074 1128.9214
1236.8975 1342.2631 1406.2300
1445.6320 1545.7405 1638.2927
1693.1892 1854.9602 2161.2653
3224.5949 3280.0622 3667.8184

ts3g

Cartesian coordinates

C	-1.834256	0.061631	0.157599
C	-1.129507	1.205060	0.160850
N	0.229565	1.164331	0.034642
C	0.972504	-0.023573	-0.070833
N	0.257462	-1.206807	0.050214
C	-1.076301	-1.168225	0.035984
O	2.169123	0.029575	-0.228019
H	-2.910731	0.045698	0.230882
H	-1.573702	2.187295	0.264285
H	0.776038	2.010824	0.033907
H	-1.567364	-2.090422	0.329628
N	-1.234256	-1.639279	-1.884183
H	-0.837909	-0.812824	-2.343773
H	-0.497619	-2.347211	-1.967197

Vibrational frequencies

-512.0894 101.0327 130.0420
208.4580 257.0401 402.1604
499.2385 528.7377 577.0075
623.5109 669.6005 738.1110
772.6833 787.2122 813.1942
857.6617 971.4755 989.2491
1015.4960 1073.1658 1122.3439
1181.3169 1239.9165 1374.8943
1425.0321 1465.6985 1547.9832
1551.1698 1703.7911 1827.6456
3181.7906 3224.9248 3263.9869
3425.0983 3527.1090 3670.0482

ts3h

Cartesian coordinates

C	-0.995721	1.167097	-0.102625
C	0.242724	1.690337	-0.034960
N	1.318585	0.870535	0.065184
C	1.244071	-0.545147	0.020319
N	-0.010733	-1.083519	-0.106559
C	-1.080359	-0.288412	-0.053180
O	2.269918	-1.180578	0.074465

N	-2.280235	-0.873881	-0.396199
H	-1.880794	1.781941	-0.169596
H	0.438499	2.755041	-0.055428
H	2.253700	1.242797	0.110379
H	-1.137331	-0.254507	1.575517
H	-2.287386	-1.875417	-0.277080
H	-3.118968	-0.406324	-0.093542

Vibrational frequencies

-1194.4878	127.8373	186.2736
333.3203	383.5906	422.8350
445.1302	499.5834	545.7403
576.8353	590.8520	634.0261
665.3539	731.9298	762.7276
789.5990	830.0761	940.7216
968.0528	988.4651	1122.5579
1131.7515	1222.5484	1255.5760
1352.5893	1449.2286	1484.6002
1554.6141	1646.2091	1706.0344
1836.7988	3225.3777	3249.3434
3606.8088	3669.4768	3723.8458

Products

uracil

Cartesian coordinates

C	-1.226502	0.360733	0.000000
C	1.269478	0.391886	0.000000
C	1.232878	-1.063498	0.000000
C	0.054343	-1.697052	0.000000
H	2.167515	-1.597605	0.000000
H	-0.026601	-2.774326	0.000000
O	2.263338	1.077951	0.000000
O	-2.281539	0.944979	0.000000
N	0.000000	0.984413	0.000000
H	-0.022861	1.992479	0.000000
N	-1.134445	-1.019971	0.000000
H	-2.012509	-1.507506	0.000000

Vibrational frequencies

152.3638	168.4213	395.0022
404.5172	526.2850	551.8673
568.3468	572.5458	691.9594
744.1432	781.4859	788.3938
837.9704	981.8472	1001.1041
1003.2726	1105.2477	1222.5016
1248.3986	1402.4559	1431.0486
1439.5315	1525.4389	1712.2336
1823.0211	1851.1506	3227.9009
3270.6979	3642.5177	3687.1617

cytosine

Cartesian coordinates

C	-1.108498	0.253983	0.015091
C	-1.068611	-1.095563	-0.006010
N	0.119978	-1.736392	-0.015393
C	1.371955	-1.065606	-0.004899
N	1.321295	0.301715	0.013469
C	0.166798	0.921712	0.026392
O	2.380271	-1.731692	-0.015688
N	0.193228	2.274536	0.069895
H	-2.044098	0.793844	0.029856
H	-1.958492	-1.713206	-0.015332
H	0.174299	-2.742176	-0.030988
H	1.091174	2.720447	-0.007365
H	-0.639300	2.818400	-0.059028

Vibrational frequencies

135.0267	139.3131	201.4701
364.9294	401.7229	539.5683
544.1434	550.9125	584.0574
642.1210	739.9186	778.9506
782.9578	804.6522	939.3014
970.2335	996.3239	1107.4038
1136.1761	1231.3447	1288.2052
1372.4492	1464.9064	1529.4895
1603.6467	1646.6829	1729.2615
1844.1652	3219.4621	3240.9381
3645.7508	3670.9008	3782.7224

pyrimidin-2-ol → ts3c → pyrimidin-2(*1H*)-one pathway with H_2O solvent molecules

pyrimidin-2-ol + 1 H_2O
Cartesian coordinates

C	2.194858	-0.577298	-0.074968
C	1.367557	-1.694235	-0.132583
N	0.045715	-1.622186	-0.098193
C	-0.471959	-0.396990	-0.003098
N	0.224501	0.749219	0.052134
C	1.551575	0.642085	0.018044
O	-1.787791	-0.330996	0.037176
H	3.272378	-0.658102	-0.101950
H	1.786593	-2.694123	-0.210015
H	2.107076	1.574040	0.067127
H	-2.064866	0.608208	0.115885
O	-2.043846	2.376223	0.193657
H	-1.081383	2.234224	0.189532
H	-2.244273	2.793144	-0.645281

Vibrational frequencies

72.8248	165.7987	186.7977
220.3766	327.2868	360.6644
427.0427	521.0114	542.6537
610.3349	661.5796	752.0642
820.4947	843.0469	903.6059

908.9191	1006.0449	1018.0308
1024.1786	1107.9931	1124.0312
1251.5128	1299.4267	1409.3238
1444.8509	1514.2388	1539.3973
1648.3191	1660.6407	1688.3272
3179.4330	3187.6038	3237.5001
3465.1261	3669.4005	3950.4400

ts3c + 1 H_2O

Cartesian coordinates

C	1.792182	0.065498	-0.019681
C	0.965550	-1.065927	-0.074103
N	-0.349626	-1.032155	-0.050751
C	-0.931344	0.184112	0.033287
N	-0.186241	1.337622	0.079010
C	1.145849	1.274169	0.057175
O	-2.193363	0.302860	0.072689
H	2.869466	-0.010680	-0.038143
H	1.410155	-2.056688	-0.140958
H	1.674041	2.220649	0.103050
H	-2.418128	1.522007	0.159301
O	-2.177220	2.674869	0.234546
H	-1.030709	2.298397	0.145790
H	-2.474926	3.129266	-0.555029

Vibrational frequencies

-1626.1640	111.8042	175.9137
365.6149	414.7879	481.2963
517.7317	547.4438	604.4827
625.5270	674.5493	746.6756
805.0210	839.5186	903.6802
996.7713	1009.9268	1020.7822
1081.8399	1152.2347	1225.8971
1247.3164	1323.8122	1411.1565
1429.6138	1499.7821	1517.1082
1589.6092	1627.4545	1705.2544
1751.7133	2005.1102	3167.1664
3203.4512	3250.2118	3930.0552

pyrimidin-2(*1H*)-one + 1 H_2O

Cartesian coordinates

C	2.203313	-0.515810	-0.061950
C	1.375219	-1.665475	-0.124862
N	0.072881	-1.659992	-0.104164
C	-0.585763	-0.453365	-0.010155
N	0.210507	0.701229	0.035642
C	1.556202	0.676544	0.016961
O	-1.799676	-0.346125	0.033124
H	3.280445	-0.584256	-0.079196
H	1.841824	-2.646762	-0.198417
H	2.057707	1.635461	0.067173
H	-2.289081	1.467275	0.224523

O	-2.002322	2.398060	0.201716
H	-0.316020	1.580064	0.090053
H	-2.398864	2.757740	-0.592122

Vibrational frequencies

67.9319	141.6363	169.6639
205.6331	278.9769	397.0153
404.6932	515.5851	529.0596
589.8042	645.0515	747.7837
789.9379	820.5794	871.8183
936.4040	1002.0841	1010.4331
1011.8698	1051.8286	1140.2605
1192.5178	1273.4083	1411.9022
1478.4722	1530.1237	1624.5469
1675.1194	1712.0536	1806.7115
3155.4704	3223.1735	3252.7412
3379.5941	3643.4145	3954.7972

pyrimidin-2-ol + 2 H_2O

Cartesian coordinates

C	2.533904	0.616214	0.098698
C	2.524489	-0.766996	-0.058814
N	1.415245	-1.482415	-0.135576
C	0.263661	-0.807210	-0.056237
N	0.155248	0.525720	0.067401
C	1.292952	1.217188	0.151203
O	-0.822818	-1.536051	-0.112707
H	3.450894	1.183915	0.167519
H	3.454195	-1.326441	-0.126474
H	1.186927	2.292854	0.262748
H	-1.649835	-1.006150	0.022007
O	-3.149976	-0.306507	0.228394
H	-1.301322	1.631947	-0.018147
H	-3.814888	-0.551322	-0.414672
O	-2.122928	2.159942	-0.112758
H	-3.025985	0.659940	0.146551
H	-2.112952	2.471798	-1.018086

Vibrational frequencies

32.6736	67.9807	104.0262
179.9446	188.0809	228.3121
271.1276	287.6821	319.1849
381.2252	435.0263	515.8894
546.4917	578.8478	613.1873
665.5924	728.1864	819.9486
843.0510	911.0971	931.6720
980.7259	1016.7478	1020.5661
1025.8815	1108.9841	1130.5576
1252.4654	1296.9559	1409.6539
1437.7994	1506.3729	1555.9858
1639.4862	1664.9551	1685.7345
1702.9200	3175.2064	3183.5579

3247.2214	3297.1757	3471.5142
3581.3372	3949.6681	3964.9207

ts3c + 2 H_2O

Cartesian coordinates

C	2.183647	0.786077	0.104750
C	2.117128	-0.605548	-0.051247
N	0.999558	-1.285402	-0.161267
C	-0.171202	-0.595418	-0.118044
N	-0.181143	0.772583	-0.013779
C	0.975098	1.433498	0.106451
O	-1.256885	-1.233371	-0.180920
H	3.121554	1.312903	0.203048
H	3.033039	-1.192397	-0.089536
H	0.893952	2.512300	0.202784
H	-2.394940	-0.676658	0.047205
O	-3.363071	-0.134770	0.218463
H	-1.314117	1.469005	-0.085975
H	-4.013115	-0.443568	-0.413191
O	-2.347393	1.985048	-0.131497
H	-3.017614	0.973545	0.028904
H	-2.475953	2.360335	-1.003518

Vibrational frequencies

-1409.7797	47.4052	86.5566
135.7929	174.9493	363.9186
399.3143	418.1552	454.6038
493.4757	539.6429	572.7833
623.4291	640.0004	687.1454
699.5171	800.7328	811.0120
842.5496	926.7113	1003.1700
1013.1354	1026.3970	1076.9722
1134.9744	1155.3890	1229.3000
1311.0842	1324.3120	1396.5286
1431.1127	1493.5353	1514.3208
1548.2204	1602.4263	1673.6058
1707.6557	1741.3949	1823.2375
1916.5565	3160.2700	3189.5543
3249.8396	3936.4688	3948.4391

pyrimidin-2(*1H*)-one + 2 H_2O

Cartesian coordinates

C	2.596231	0.605454	0.205700
C	2.517722	-0.798906	0.043889
N	1.417307	-1.476549	-0.128585
C	0.218191	-0.801273	-0.152888
N	0.267706	0.589029	-0.033419
C	1.412099	1.272196	0.150687
O	-0.860012	-1.364342	-0.275462
H	3.536480	1.114564	0.354120
H	3.435295	-1.385257	0.059340
H	1.314686	2.346893	0.247639

H	-2.463779	-0.829491	0.206059
O	-3.295067	-0.355854	0.408551
H	-0.626915	1.106491	-0.095434
H	-3.967325	-0.783093	-0.121132
O	-2.136583	1.989137	-0.180266
H	-2.728693	1.253821	0.089885
H	-2.410225	2.210744	-1.070688

Vibrational frequencies

27.7045	66.5847	81.4802
146.6791	202.0949	209.7950
260.3597	288.2023	313.3222
401.6972	418.0476	506.2090
529.1735	530.1712	599.9347
647.1076	694.9003	788.4242
825.8925	882.5123	935.8128
987.8291	1010.4972	1011.8979
1055.4377	1074.5535	1139.8102
1198.9834	1276.5839	1414.9399
1483.0944	1540.2418	1638.3042
1684.4044	1700.1537	1712.8936
1794.5963	3155.8030	3204.6616
3224.5227	3265.0696	3483.4174
3580.1318	3950.7435	3965.1297

pyrimidin-2-ol + 3 H_2O

Cartesian coordinates

C	-2.766926	0.930079	-0.145412
C	-3.041740	-0.430499	-0.253928
N	-2.116729	-1.370172	-0.155363
C	-0.864929	-0.952713	0.062064
N	-0.491733	0.328735	0.204910
C	-1.446558	1.253296	0.091121
O	0.042042	-1.892703	0.139819
H	-3.536382	1.683319	-0.237559
H	-4.055836	-0.780456	-0.430387
H	-1.115047	2.282744	0.196329
H	0.954659	-1.524854	0.257120
O	2.552900	-1.158752	0.486490
H	1.018233	1.265467	0.514959
H	2.785987	-0.859412	1.364583
O	1.664929	1.997345	0.635865
H	2.989060	1.513472	-0.446604
H	1.743413	2.120222	1.581108
O	3.555033	0.898429	-0.949958
H	2.986400	-0.526157	-0.123393
H	4.449392	1.230788	-0.887434

Vibrational frequencies

22.9607	37.8891	63.1592
89.1414	93.6114	171.9514
180.7971	196.9857	213.0858

254.4759	270.7869	305.1396
310.1152	386.3424	432.5810
454.4399	527.5713	540.8290
551.9098	613.2809	664.3853
711.5038	819.4706	836.4719
844.7019	914.5755	954.8810
1019.5387	1025.4499	1025.6931
1056.3801	1109.3805	1128.9738
1247.9247	1293.6410	1406.6564
1418.0162	1498.9626	1557.1658
1640.9586	1659.4500	1682.4722
1688.8254	1695.3169	3168.3463
3178.6658	3241.0858	3307.8883
3416.4863	3531.2864	3622.0145
3966.0223	3969.7522	3973.9671

ts3c + 3 H_2O

Cartesian coordinates

C	3.448860	0.897706	0.568066
C	3.632069	-0.330794	-0.078770
N	2.657595	-1.063993	-0.567105
C	1.381709	-0.599844	-0.432797
N	1.130021	0.610980	0.162403
C	2.146380	1.327134	0.647918
O	0.425483	-1.286984	-0.873280
H	4.273508	1.473870	0.962397
H	4.635716	-0.735124	-0.202770
H	1.878557	2.276109	1.105322
H	-0.789214	-1.492461	-0.262477
O	-1.692689	-1.743703	0.240926
H	-0.144561	1.225442	0.132860
H	-1.476739	-2.425933	0.877304
O	-1.102861	1.757088	0.111323
H	-2.008335	1.013850	0.656479
H	-1.282655	1.953019	-0.809255
O	-2.683053	0.246746	1.112071
H	-2.250746	-0.749689	0.732453
H	-3.586421	0.365666	0.816379

Vibrational frequencies

-1007.2094	31.3489	36.1398
66.5445	76.3020	117.7897
169.0246	301.3284	354.2104
379.1143	419.4049	445.8449
487.8424	545.5112	558.4610
580.4309	621.7515	655.1088
656.6013	681.9493	713.7170
806.0618	811.3033	850.6238
917.9770	1015.1033	1025.3273
1036.0671	1091.4655	1128.2925
1172.3739	1218.5236	1282.0541
1319.7121	1374.2103	1428.6104

1447.0464	1502.4380	1546.1406
1604.4630	1617.5334	1653.3312
1686.7490	1702.8187	1772.0809
1808.9140	1906.6384	2179.0798
3144.9502	3178.8036	3245.0551
3937.8147	3944.4047	3947.4623

pyrimidin-2(*1H*)-one + 3 H_2O
Cartesian coordinates

C	-2.817497	0.978800	-0.256632
C	-3.031566	-0.420451	-0.257310
N	-2.114733	-1.323831	-0.045692
C	-0.822775	-0.916446	0.196226
N	-0.588240	0.456704	0.226340
C	-1.543071	1.377440	0.002518
O	0.096816	-1.700225	0.385000
H	-3.614412	1.682527	-0.443217
H	-4.034354	-0.801678	-0.445252
H	-1.211811	2.407886	0.048670
H	1.824021	-1.572297	0.263892
O	2.792909	-1.440216	0.303901
H	0.357305	0.811045	0.433825
H	3.026678	-1.625771	1.212527
O	1.597829	2.057661	0.689709
H	2.328150	1.802878	0.084397
H	1.991883	2.077220	1.561592
O	3.427866	0.897787	-0.839524
H	3.302661	-0.006017	-0.479669
H	4.358621	1.001806	-1.027702

Vibrational frequencies

23.8038	30.8800	38.1086
56.0887	86.0127	139.1152
155.8374	188.0910	202.2041
206.3294	294.8373	305.1141
327.5947	405.1725	413.5274
464.1870	504.3836	518.3271
539.6945	604.4337	650.2819
757.5168	794.2376	827.2507
832.1586	886.0714	945.7279
1001.1521	1011.1669	1029.2397
1054.0586	1089.4855	1145.4674
1202.1687	1261.3908	1398.8573
1475.7449	1519.1406	1624.7974
1666.1875	1690.2741	1704.5028
1709.3250	1783.5063	3152.2474
3226.0633	3252.5086	3289.5673
3453.4161	3524.9647	3572.5859
3959.5326	3969.8660	3983.1358

pyrimidin-2-ol + 4 H_2O
Cartesian coordinates

C	-3.195145	0.688525	-0.196796
C	-3.402085	-0.685709	-0.132920
N	-2.429024	-1.558404	0.076817
C	-1.204676	-1.050015	0.231585
N	-0.893520	0.252776	0.218908
C	-1.893849	1.107307	-0.002052
O	-0.242612	-1.926244	0.415353
H	-4.002250	1.384410	-0.376794
H	-4.397291	-1.104783	-0.257406
H	-1.616606	2.157664	-0.011951
H	0.642584	-1.495090	0.416532
O	2.330622	-1.173361	0.261121
H	0.509682	1.386217	0.677265
H	2.813812	-1.994721	0.361196
O	0.977028	2.203863	0.942340
H	2.693077	1.979477	0.451720
H	0.838306	2.269633	1.887403
O	3.527957	1.531668	0.219721
H	3.215614	0.836698	-1.383722
H	3.430653	0.685442	0.669800
O	2.921543	0.131472	-1.999180
H	2.500085	-0.866436	-0.659245
H	3.669321	-0.051685	-2.567229

Vibrational frequencies

23.0375	31.6491	52.9847
69.3425	78.6320	87.4093
143.4618	169.8528	190.1212
200.9031	255.2701	269.7901
290.3731	299.5023	309.6281
361.4037	398.6604	414.5245
439.1538	464.2093	535.9123
544.6085	554.0340	592.1216
613.1528	663.6152	729.0723
820.7923	828.7469	846.2392
911.0848	922.4168	935.3578
1025.4859	1029.1681	1040.0721
1061.4102	1110.5846	1128.0023
1252.6550	1295.0935	1407.6442
1423.8971	1501.1736	1551.2242
1646.1448	1666.1283	1673.6427
1685.3233	1697.7024	1717.6328
3178.0621	3181.0154	3245.4363
3378.1735	3458.0828	3515.1774
3545.1562	3646.3155	3862.7288
3944.8556	3955.0948	3963.5415

ts3c + 4 H_2O

Cartesian coordinates

C	-2.445295	0.860007	-0.542896
C	-2.613743	-0.503918	-0.275485
N	-1.672193	-1.288152	0.196363

C	-0.443092	-0.736813	0.436538
N	-0.222689	0.610062	0.266971
C	-1.205044	1.363923	-0.223840
O	0.496363	-1.471068	0.823131
H	-3.238473	1.475713	-0.942566
H	-3.578558	-0.976981	-0.456516
H	-0.971484	2.419712	-0.352221
H	1.846520	-1.289081	0.413013
O	2.816010	-1.322116	0.017503
H	0.962732	1.358301	0.893172
H	2.974494	-2.251816	-0.148165
O	1.714519	1.957533	1.297229
H	2.902962	2.038245	0.568050
H	1.307707	2.716927	1.710844
O	3.802009	1.926825	0.025273
H	3.533175	1.201704	-0.891799
H	4.396418	1.459089	0.617277
O	3.156949	0.386865	-1.680337
H	2.974643	-0.452103	-1.046520
H	3.795653	0.168978	-2.359712

Vibrational frequencies

-620.6199	22.3858	24.5672
40.4902	63.3739	77.0622
88.1501	102.4729	162.3097
208.1168	263.7385	330.7580
358.8677	427.0896	445.0111
472.4315	478.3408	546.0464
549.0992	605.5777	608.9538
634.8968	640.6455	671.6204
689.0992	713.2219	784.8219
825.8828	851.7491	911.5113
1004.0567	1018.4118	1024.8563
1077.2839	1085.2472	1117.8358
1153.0748	1211.1158	1227.0349
1314.7483	1334.5479	1416.3223
1484.4560	1567.4009	1592.8490
1609.4769	1656.4414	1679.8652
1737.2250	1749.0811	1781.5945
1819.3687	2072.6630	2162.0149
2427.4911	2480.1538	3141.0223
3147.0390	3242.2117	3911.4118
3947.8986	3950.5466	3976.2982

pyrimidin-2(*1H*)-one + 4 H_2O

Cartesian coordinates

C	-2.629614	0.690553	-0.858784
C	-2.669437	-0.720674	-0.861756
N	-1.830801	-1.500298	-0.231747
C	-0.818197	-0.926386	0.494175
N	-0.782184	0.460022	0.554309
C	-1.634312	1.249674	-0.115382

O	0.036876	-1.580733	1.085767
H	-3.340042	1.287655	-1.410181
H	-3.449486	-1.227717	-1.428074
H	-1.465703	2.314633	-0.012499
H	1.673874	-1.462221	0.730282
O	2.537786	-1.374104	0.267425
H	-0.016514	0.916506	1.078832
H	2.956982	-2.232435	0.316669
O	1.114936	2.122274	1.602541
H	1.887064	1.953626	1.014813
H	1.454912	2.098571	2.496524
O	3.051433	1.348754	-0.090077
H	2.547722	1.234022	-0.909079
H	3.179032	0.429478	0.188251
O	1.292735	0.007162	-1.795585
H	1.689059	-0.708954	-1.273864
H	1.164888	-0.342777	-2.676163

Vibrational frequencies

25.2295	32.7820	47.9563
51.8128	65.8807	89.7042
138.7048	157.3194	164.4774
194.7307	217.2170	243.7831
265.9058	296.6549	307.8718
311.0167	381.3137	414.8147
456.1792	488.6454	514.5355
519.9418	538.0645	604.2402
613.4721	652.4889	677.2180
751.4504	802.1446	829.5730
860.4446	894.7014	923.0493
1002.8649	1014.2465	1022.6295
1063.8411	1110.9249	1144.2755
1211.4783	1268.1088	1407.6187
1480.7424	1530.1836	1633.7985
1649.2478	1674.9577	1704.3493
1707.1488	1741.3831	1772.1300
3150.6502	3222.4335	3231.3677
3258.8721	3419.9916	3442.6749
3696.8794	3751.8157	3789.7668
3962.9616	3967.7721	3974.1939

2) SCRF/PCM//ωB97X-D/6-311G(d,p) for pyrimidin-2-ol → ts3c → pyrimidin-2(1H)-one pathway with H_2O solvent molecules

pyrimidin-2-ol + 0 H_2O

Cartesian coordinates

C	-1.259893	0.710530	0.110981
C	-1.269782	-0.676598	0.104156
N	-0.159938	-1.406808	0.005815
C	0.969929	-0.714308	-0.086362
N	1.110873	0.608200	-0.091030
C	-0.016052	1.312450	0.008617

O	2.081736	-1.447851	-0.184880
H	-2.169412	1.288517	0.191460
H	-2.201020	-1.229487	0.180230
H	0.088935	2.392728	0.005665
H	2.824627	-0.837372	-0.244656

Vibrational frequencies

193.4801	418.0399	463.3364
524.6721	554.3584	607.4514
656.5607	816.7769	838.9126
903.9870	1017.4628	1021.7668
1024.8470	1112.4002	1112.9066
1213.3172	1263.4007	1371.4242
1388.3202	1487.6380	1506.8919
1654.7366	1665.0558	3195.2346
3199.7800	3252.8200	3855.0096

ts3c + 0 H_2O

Cartesian coordinates

C	1.754563	0.038582	-0.007183
C	1.056489	-1.158422	0.054304
N	-0.267101	-1.102068	0.095696
C	-0.917763	0.095364	0.078291
N	-0.324383	1.283451	0.020494
C	1.010007	1.217393	-0.020973
O	-2.161667	-0.204426	0.128696
H	2.833447	0.057595	-0.043034
H	1.532342	-2.131043	0.070198
H	1.524450	2.172589	-0.068662
H	-1.519243	-1.385820	0.145873

Vibrational frequencies

-1993.1438	175.9924	407.2203
499.5223	562.7114	614.8237
707.4814	795.8918	797.7777
935.9356	1011.5300	1027.5089
1038.6746	1087.8314	1116.3360
1143.4585	1244.5780	1299.2834
1408.9034	1487.7115	1565.9726
1629.9702	1679.0692	2161.5292
3186.3576	3232.4502	3260.7857

pyrimidin-2(*1H*)-one + 0 H_2O

Cartesian coordinates

C	-1.056325	0.789683	0.002435
C	-1.028657	-0.569561	0.000554
N	0.162347	-1.202203	-0.001841
C	1.398606	-0.546197	-0.002545
N	1.360690	0.832238	-0.000625
C	0.200569	1.436361	0.001691
O	2.427710	-1.197727	-0.004757
H	-1.983371	1.341806	0.004381

H	-1.910489	-1.196261	0.000841
H	0.197617	-2.212124	-0.003258
H	0.231304	2.523984	0.003128

Vibrational frequencies

147.5031	403.2068	497.8972
501.1904	587.3812	643.6012
731.1390	788.9272	828.1678
867.2811	1005.5601	1012.4055
1026.9816	1057.0621	1128.9958
1190.3345	1240.8700	1388.2324
1464.4607	1502.2444	1607.5580
1701.2036	1772.9483	3168.1990
3248.9840	3271.2051	3630.9436

pyrimidin-2-ol + 1 H_2O

Cartesian coordinates

C	2.197189	-0.582062	-0.082386
C	1.372459	-1.697595	-0.133509
N	0.045133	-1.620715	-0.093723
C	-0.463912	-0.393475	0.000042
N	0.230142	0.749075	0.056192
C	1.557920	0.641110	0.014359
O	-1.786522	-0.322947	0.041357
H	3.273991	-0.664545	-0.115849
H	1.791916	-2.696318	-0.210032
H	2.116216	1.570445	0.060437
H	-2.055150	0.622970	0.099200
O	-2.061953	2.370521	0.192282
H	-1.096131	2.259151	0.163568
H	-2.293647	2.760816	-0.653559

Vibrational frequencies

67.5340	122.6414	190.4403
212.3801	311.9360	368.9381
422.2898	506.6394	540.7078
609.2128	657.3647	692.6911
825.3870	841.6370	880.1274
904.6806	1016.7002	1024.1957
1027.4587	1111.9906	1123.3027
1249.6742	1291.7230	1396.1825
1439.4503	1492.1002	1526.3261
1643.4194	1654.7203	1674.8076
3191.2627	3200.5002	3245.4585
3398.3538	3658.6982	3923.9999

ts3c + 1 H_2O

Cartesian coordinates

C	1.792422	0.059649	-0.028095
C	0.974045	-1.070383	-0.075328
N	-0.348780	-1.034406	-0.041528
C	-0.923748	0.181926	0.045148

N	-0.186940	1.333210	0.096232
C	1.143875	1.270772	0.059679
O	-2.195637	0.294693	0.084063
H	2.869396	-0.013146	-0.058589
H	1.420332	-2.059062	-0.145074
H	1.673023	2.215927	0.102588
H	-2.425434	1.545638	0.149238
O	-2.185955	2.672943	0.232690
H	-1.070068	2.323642	0.162711
H	-2.440848	3.122598	-0.577551

Vibrational frequencies

-1543.2420	110.4834	183.9641
368.7233	414.9357	459.9537
528.9064	563.7956	605.0117
630.2965	659.8007	715.6342
812.5763	841.9224	898.1769
928.1089	1010.3265	1030.0920
1060.8274	1102.2872	1146.5638
1237.8311	1317.3958	1397.7806
1419.8297	1496.6079	1523.2697
1575.6507	1612.5204	1685.3339
1711.5368	2033.3509	3178.9961
3215.5623	3255.4710	3896.2617

pyrimidin-2(*1H*)-one + 1 H_2O

Cartesian coordinates

C	2.205844	-0.522053	-0.078515
C	1.383642	-1.666732	-0.132111
N	0.073183	-1.655876	-0.096244
C	-0.573250	-0.450330	0.002442
N	0.215754	0.695982	0.051288
C	1.560795	0.673607	0.014032
O	-1.797836	-0.348061	0.048966
H	3.282269	-0.589402	-0.110883
H	1.848217	-2.647036	-0.210599
H	2.061229	1.631845	0.060864
H	-2.283011	1.470100	0.157435
O	-2.042444	2.412767	0.188686
H	-0.300436	1.578491	0.115421
H	-2.263241	2.747506	-0.682893

Vibrational frequencies

66.9532	144.8245	157.1925
204.6458	330.5614	361.0789
407.2229	516.5346	528.6958
593.3196	649.6352	745.2274
800.8049	824.1430	881.8249
917.2861	1014.4537	1015.6982
1026.2661	1068.3664	1139.6692
1209.6734	1267.3601	1401.2267
1476.6988	1519.9626	1619.9964

1653.4078	1697.7887	1744.1969
3172.6229	3240.1557	3261.3528
3402.2790	3646.0258	3927.9137

pyrimidin-2-ol + 2 H_2O
Cartesian coordinates

C	2.534765	0.625582	-0.042012
C	2.533496	-0.763378	-0.027829
N	1.420389	-1.487141	-0.000110
C	0.271117	-0.806935	0.014617
N	0.155787	0.526893	0.006600
C	1.291847	1.227738	-0.022053
O	-0.817854	-1.547016	0.042719
H	3.449173	1.200319	-0.064499
H	3.465358	-1.321210	-0.039431
H	1.186287	2.308135	-0.027484
H	-1.652494	-1.007083	0.019763
O	-3.168211	-0.335058	-0.043964
H	-1.309450	1.641329	0.103931
H	-3.534816	-0.445063	-0.923903
O	-2.143298	2.155028	0.150073
H	-3.007558	0.627232	0.048319
H	-2.198312	2.610592	-0.692492

Vibrational frequencies

27.2018	63.4658	107.3123
173.3699	192.6173	227.3018
275.6833	294.7510	363.3820
389.5935	432.4187	522.3222
540.0987	545.3339	612.9859
664.6967	703.9235	824.6869
840.6788	908.6772	960.1077
981.6915	1018.3390	1023.7569
1027.3633	1113.1389	1131.0498
1248.9101	1287.5472	1399.7409
1418.5961	1493.4614	1529.3785
1642.0578	1659.2975	1669.9711
1686.6457	3188.9530	3189.9938
3222.7254	3257.1351	3460.4724
3536.5679	3924.2822	3927.4689

ts3c + 2 H_2O
Cartesian coordinates

C	2.209077	0.779397	-0.001595
C	2.153396	-0.614669	-0.020717
N	1.030871	-1.309130	-0.014253
C	-0.144280	-0.619171	0.013109
N	-0.166430	0.750631	0.027110
C	0.989183	1.417531	0.021406
O	-1.226263	-1.272613	0.028264
H	3.143545	1.321187	-0.005988
H	3.072873	-1.195883	-0.043334

H	0.912661	2.500875	0.035665
H	-2.494701	-0.685222	0.023623
O	-3.428577	-0.177243	0.025950
H	-1.419617	1.522101	0.035703
H	-3.886124	-0.390672	-0.791574
O	-2.396851	1.968592	0.058585
H	-3.048280	0.958880	0.015237
H	-2.511938	2.483570	-0.744560

Vibrational frequencies

-944.9058	34.4524	76.2920
135.4315	175.1242	291.1830
371.8194	418.9049	455.9982
524.6797	538.3340	571.2706
615.8095	636.0951	667.2854
681.0047	809.4530	825.6600
845.4713	912.5490	1008.1437
1019.5424	1032.0352	1094.3983
1112.7610	1146.3457	1213.9733
1277.5164	1322.4525	1422.1101
1465.5552	1486.8142	1539.5972
1596.6302	1645.4392	1679.4494
1694.5082	1857.2211	1979.7168
2133.4557	3164.3545	3188.4484
3245.8370	3900.9615	3903.7060

pyrimidin-2(*1H*)-one + 2 H_2O

Cartesian coordinates

C	2.602414	0.660796	0.012630
C	2.551396	-0.746820	-0.020617
N	1.449768	-1.458068	-0.031099
C	0.242708	-0.807249	-0.007466
N	0.261295	0.579839	0.016452
C	1.398817	1.298631	0.028742
O	-0.828728	-1.414220	-0.006322
H	3.536582	1.200837	0.022044
H	3.481051	-1.311061	-0.040633
H	1.283884	2.374803	0.051192
H	-2.491275	-0.854989	0.036626
O	-3.376292	-0.437736	0.038245
H	-0.645453	1.081034	0.021375
H	-3.738412	-0.628409	-0.829238
O	-2.159118	1.984823	0.040401
H	-2.759826	1.210421	0.064252
H	-2.300186	2.380865	-0.822030

Vibrational frequencies

29.7017	68.2282	86.4053
163.8642	187.3139	205.2170
269.1713	288.6283	359.5476
395.4119	414.7761	520.2759
524.0632	533.2837	601.7450

647.9194	693.5162	804.7767
827.2260	889.1163	921.2100
980.1660	1012.5653	1024.2632
1047.4823	1070.6440	1140.6928
1212.3792	1273.6511	1407.4517
1482.3368	1537.9740	1634.2600
1664.9927	1679.2873	1700.2855
1737.1492	3172.0894	3186.2670
3233.6376	3260.2084	3486.0233
3561.1785	3925.9269	3930.0713

pyrimidin-2-ol + 3 H_2O

Cartesian coordinates

C	-2.824807	0.893852	-0.035635
C	-3.059788	-0.457242	-0.257626
N	-2.096075	-1.371201	-0.256699
C	-0.858500	-0.925528	-0.025896
N	-0.518888	0.349579	0.195565
C	-1.507751	1.246055	0.186659
O	0.083342	-1.844865	-0.025213
H	-3.621820	1.623138	-0.040262
H	-4.065461	-0.822052	-0.445098
H	-1.212575	2.275926	0.362473
H	0.978978	-1.463228	0.180342
O	2.539897	-1.140559	0.553580
H	1.023696	1.331500	0.398532
H	2.633644	-0.783558	1.438704
O	1.676910	2.062707	0.419284
H	3.033420	1.444519	-0.517463
H	1.893162	2.181980	1.345755
O	3.668566	0.830160	-0.939664
H	3.010311	-0.507156	-0.030097
H	4.529907	1.084151	-0.602913

Vibrational frequencies

30.2685	46.7154	86.2953
90.4821	110.3923	168.3564
197.5483	208.3591	268.0049
282.1300	292.2107	326.8354
371.9433	400.8616	437.7467
499.5693	530.3966	534.8821
552.7175	613.6792	663.6159
716.5949	831.8162	842.5639
845.1716	911.2480	965.8583
1027.0124	1038.3755	1040.7154
1048.2179	1115.2133	1127.5849
1246.9665	1286.4337	1404.9319
1406.5698	1492.8264	1528.9907
1643.7862	1657.9912	1669.9864
1676.3299	1686.8977	3185.3412
3190.2888	3200.6483	3255.0972
3446.2905	3485.0595	3554.2401

3930.1500 3933.7785 3937.0121

ts3c + 3 H_2O
Cartesian coordinates

C	-2.636249	0.876569	-0.062976
C	-2.779317	-0.505708	-0.181606
N	-1.771472	-1.357118	-0.164262
C	-0.504777	-0.853009	-0.020767
N	-0.289454	0.497125	0.101366
C	-1.337374	1.318961	0.076715
O	0.462433	-1.654572	-0.006304
H	-3.479157	1.552131	-0.081371
H	-3.769706	-0.942990	-0.298260
H	-1.109450	2.377984	0.174269
H	1.949739	-1.437683	0.209536
O	2.957117	-1.391720	0.342046
H	1.055510	1.308167	0.231090
H	3.109468	-1.422884	1.288906
O	1.854977	1.958889	0.274405
H	2.938504	1.351411	-0.240455
H	1.979703	2.183119	1.199520
O	3.719067	0.706434	-0.638810
H	3.469359	-0.249349	-0.216613
H	4.583269	0.991161	-0.326542

Vibrational frequencies

-241.2094	24.0304	43.9701
77.1573	85.0291	117.7366
164.5618	246.2963	302.4786
405.5529	410.2730	432.6434
487.2934	501.2953	545.8454
560.0198	579.5083	630.4777
668.2048	693.9127	783.0147
806.2544	847.7642	907.9518
962.4263	1015.6925	1024.3918
1030.8395	1088.0730	1096.6143
1118.7629	1200.9756	1232.9873
1308.0620	1389.3032	1415.0648
1452.4387	1485.9318	1590.2675
1596.6909	1664.2990	1669.6052
1683.1044	1771.8959	1838.0519
2058.0910	2525.4921	2799.5216
3149.7374	3171.3277	3251.7313
3889.0816	3916.1730	3922.4143

pyrimidin-2(*1H*)-one + 3 H_2O
Cartesian coordinates

C	-2.870580	0.965358	-0.116531
C	-3.069199	-0.421981	-0.261342
N	-2.122073	-1.327433	-0.201229
C	-0.831209	-0.919884	0.018701
N	-0.606029	0.438803	0.168216

C	-1.584872	1.359009	0.102133
O	0.106393	-1.716061	0.083934
H	-3.684494	1.671193	-0.175718
H	-4.074721	-0.797620	-0.437568
H	-1.271899	2.387229	0.231606
H	1.805629	-1.459971	0.342792
O	2.766008	-1.337936	0.489457
H	0.354665	0.786761	0.332244
H	2.841896	-1.073213	1.407858
O	1.669897	1.928432	0.533985
H	2.400954	1.643745	-0.054847
H	2.039711	1.910657	1.418557
O	3.586136	0.774878	-0.996084
H	3.385526	-0.063466	-0.528206
H	4.484541	0.996320	-0.744358

Vibrational frequencies

26.8555	41.9327	56.3003
82.9716	92.0325	168.9169
174.7104	200.1891	266.3400
276.7997	283.2864	321.0970
387.6696	399.5151	418.5318
486.9093	502.8982	525.5600
537.4333	605.7286	652.5623
734.5005	793.7307	807.2246
829.0346	892.0489	952.0967
1006.8919	1012.8394	1042.1418
1067.3906	1085.3090	1146.3736
1214.0831	1253.8052	1391.7517
1477.7137	1516.2377	1622.9948
1661.9582	1673.3092	1679.3204
1696.5855	1723.1170	3170.3319
3217.2272	3238.4195	3269.6215
3443.1107	3505.2724	3548.8995
3932.0237	3933.7207	3935.5785

pyrimidin-2-ol + 4 H_2O

Cartesian coordinates

C	-2.995304	1.063230	-0.414244
C	-3.334176	-0.278603	-0.537768
N	-2.494410	-1.267943	-0.257581
C	-1.276540	-0.913698	0.163318
N	-0.854458	0.346118	0.338736
C	-1.718005	1.320488	0.042035
O	-0.456873	-1.908031	0.420204
H	-3.689216	1.855940	-0.653188
H	-4.322724	-0.572288	-0.878606
H	-1.358287	2.334749	0.183698
H	0.471725	-1.603360	0.643814
O	2.029962	-1.329446	0.944420
H	0.623347	0.989574	1.083901
H	2.056924	-0.457700	1.369893

O	1.487718	1.317871	1.430992
H	2.446913	1.907704	0.055406
H	1.298918	1.838647	2.213208
O	2.964297	2.023399	-0.764503
H	2.473910	-1.179254	0.082822
H	3.819906	2.343589	-0.472598
O	3.196253	-0.626300	-1.424751
H	4.135160	-0.821719	-1.430566
H	3.142213	0.343874	-1.299985

Vibrational frequencies

18.5072	23.5833	40.5616
75.1959	81.3161	116.6502
173.7287	196.1712	205.4304
234.6738	251.0900	268.6413
280.2831	289.9740	293.6791
333.4357	391.3289	423.8396
500.5777	524.7918	543.7634
547.7011	585.6350	614.5002
665.1144	700.6361	720.5035
811.0723	824.7667	841.5601
892.4568	909.8440	970.4960
1019.5951	1029.5320	1035.6939
1082.5716	1114.8047	1127.9288
1249.1990	1296.4359	1407.0909
1429.1348	1494.5061	1534.1186
1642.3827	1650.4518	1674.1636
1679.3538	1682.5635	1715.1110
3034.8375	3188.6084	3191.8098
3250.2675	3325.3173	3473.0755
3540.5791	3604.2533	3715.9991
3929.4810	3933.8552	3940.2199

ts3c + 4 H_2O

Cartesian coordinates

C	-2.908023	0.998672	-0.316039
C	-3.154362	-0.347732	-0.587665
N	-2.267165	-1.310408	-0.427894
C	-1.020165	-0.968884	0.035381
N	-0.712144	0.340741	0.330002
C	-1.639693	1.278050	0.149656
O	-0.160266	-1.865966	0.189305
H	-3.656215	1.765006	-0.458540
H	-4.131268	-0.656014	-0.957649
H	-1.340001	2.295125	0.392805
H	1.387597	-1.634560	0.621938
O	2.340355	-1.457943	0.856209
H	0.664500	0.849749	0.868528
H	2.290269	-0.608476	1.317869
O	1.589614	1.204107	1.171886
H	2.408963	1.604179	0.004100
H	1.455603	1.839072	1.877858

O	2.984368	1.671725	-0.851459
H	3.084673	-1.077755	-0.461243
H	3.750984	2.224474	-0.670366
O	3.511432	-0.641750	-1.272006
H	4.445108	-0.867323	-1.265161
H	3.299445	0.620555	-1.100020

Vibrational frequencies

-240.8540	21.4174	38.2525
53.9960	77.6279	87.6398
132.0586	166.0421	190.6305
233.6329	254.1018	371.6461
379.6604	423.7435	430.8873
468.1556	475.9841	537.8979
541.8065	578.4632	615.5690
626.1916	669.2183	690.0921
710.2487	792.5703	794.5055
845.9375	902.0082	946.2081
990.3312	1009.5923	1020.4419
1024.4139	1088.5914	1097.5622
1121.8555	1158.0680	1195.4162
1213.0485	1307.9279	1388.1783
1410.9004	1480.6526	1583.5145
1606.2136	1664.6759	1683.6227
1695.4763	1737.2551	1751.1402
1868.5924	2321.1752	2623.5419
2859.0553	3149.4283	3168.0899
3192.9711	3243.8925	3764.7221
3888.8356	3912.6577	3934.6436

pyrimidin-2(*1H*)-one + 4 H_2O

Cartesian coordinates

C	-3.043640	1.094955	-0.382856
C	-3.331637	-0.268342	-0.595884
N	-2.509194	-1.258278	-0.346424
C	-1.265946	-0.974777	0.160112
N	-0.958910	0.359715	0.389902
C	-1.810706	1.368156	0.126762
O	-0.441279	-1.852435	0.410911
H	-3.756226	1.873320	-0.607652
H	-4.303282	-0.547907	-0.997102
H	-1.449482	2.365142	0.344731
H	1.296185	-1.649655	0.795290
O	2.224523	-1.398775	0.959235
H	-0.033052	0.595302	0.777618
H	2.139812	-0.511584	1.342455
O	1.511805	1.247859	1.367426
H	2.018965	1.656373	0.625989
H	1.534374	1.859582	2.104820
O	2.885771	2.011791	-0.795739
H	2.882258	-0.981739	-0.598865
H	3.752628	2.364239	-0.585394

O	3.232321	-0.602394	-1.435531
H	4.158401	-0.850541	-1.451224
H	3.055177	1.104488	-1.133205

Vibrational frequencies

15.8628	26.4867	38.4345
66.2345	82.6092	100.1469
166.3857	172.6131	186.4009
229.3253	264.0442	275.6229
282.4244	293.0308	300.8623
345.9501	409.1646	417.8532
514.6310	514.8485	529.6636
551.6002	557.4048	601.0303
648.7996	661.1280	770.9913
801.8723	813.1518	827.6375
846.4804	887.1343	982.5982
1011.6597	1016.0943	1034.3096
1050.0112	1068.5347	1141.6893
1210.4486	1262.7779	1400.3056
1479.9341	1524.9317	1626.9730
1663.8002	1669.6907	1686.4889
1697.5877	1704.7524	1742.9335
3163.0157	3231.0029	3261.3931
3263.6594	3350.3989	3426.7145
3497.5058	3608.0963	3721.4271
3930.5219	3934.0531	3945.1175

4-hydroxypyrimidin-2(1H)-one → ts3f → uracil pathway with H_2O solvent molecules

4-hydroxypyrimidin-2(*1H*)-one + H_2O
Cartesian coordinates

C	-1.956654	-1.067516	0.005195
C	-0.860185	1.099000	-0.001399
C	0.387359	-0.868865	0.001136
C	-0.769692	-1.705206	0.008118
H	-2.904606	-1.585973	0.006829
H	-0.681667	-2.777546	0.011596
O	-0.986667	2.300381	0.002144
N	-2.004716	0.281401	-0.000041
H	-2.882140	0.772689	-0.000864
N	0.341866	0.438643	-0.005491
O	1.555028	-1.475211	0.000534
H	2.271463	-0.794251	-0.008842
O	3.096628	0.729859	-0.086668
H	3.517316	1.060377	0.707058
H	2.194696	1.099671	-0.083434

Vibrational frequencies

69.6279	144.9484	154.2770
209.3295	215.8181	305.3612
389.8231	429.8068	434.9712
544.6189	579.6942	587.6844

647.4849 735.1794 747.5059
794.3897 808.6532 823.8306
949.2364 986.2546 1000.3094
1033.2978 1126.1751 1225.6115
1274.8167 1357.3800 1410.8318
1513.0240 1537.6324 1631.9319
1667.8151 1716.3909 1828.2220
3227.4753 3273.1134 3334.4242
3609.3737 3667.6489 3940.3328

ts3f + H_2O
Cartesian coordinates
C -1.806458 -1.203919 0.008228
C -0.899555 1.048163 -0.003198
C 0.540180 -0.859949 -0.000795
C -0.579604 -1.756029 0.010282
H -2.712807 -1.792365 0.012150
H -0.420906 -2.820341 0.015009
O -1.108650 2.237670 0.001055
N -1.967379 0.140669 0.001220
H -2.882164 0.557213 0.001781
N 0.339655 0.470701 -0.009976
O 1.734356 -1.296013 -0.003955
H 2.452393 -0.287470 -0.024904
O 2.716650 0.870506 -0.086641
H 3.127243 1.178561 0.722738
H 1.564082 1.017910 -0.036255

Vibrational frequencies
-1574.3869 101.1552 169.7108
195.2728 276.0381 426.1670
461.3423 534.7890 537.8666
565.2309 614.0213 628.1744
632.4018 710.8026 755.2114
800.9853 815.1331 838.6863
1004.2057 1020.2755 1046.1717
1118.7237 1184.5347 1234.5776
1326.5088 1378.8269 1403.6047
1458.4770 1512.4307 1554.3888
1618.2630 1679.8497 1735.3893
1840.1281 1998.5864 3225.3511
3272.9512 3675.8093 3914.4551

uracil + H_2O
Cartesian coordinates
C -1.981736 -1.020390 0.007483
C -0.850717 1.123468 -0.001931
C 0.427087 -0.998074 -0.001003
C -0.835492 -1.713189 0.006839
H -2.950728 -1.498154 0.011369
H -0.816209 -2.789324 0.009788
O -0.889712 2.327924 0.000184

N	-1.997883	0.343903	0.003474
H	-2.861870	0.856283	0.005617
N	0.310843	0.386451	-0.008078
O	1.524016	-1.530630	-0.002581
H	2.905890	-0.196179	-0.066701
O	3.135004	0.746604	-0.084338
H	3.633013	0.905521	0.716858
H	1.189863	0.907306	-0.019161

Vibrational frequencies

62.4273	125.9185	159.2069
169.5106	186.7106	260.3114
362.8753	413.9627	416.0152
534.0978	562.4308	574.3655
585.9024	697.0234	746.0926
782.6221	788.4626	833.5119
892.0675	1001.5334	1002.0440
1007.1786	1110.6873	1228.8129
1263.0281	1412.5703	1443.3448
1475.1115	1535.6246	1660.9928
1707.2059	1787.7302	1852.8921
3227.2668	3271.8722	3420.0124
3680.8868	3685.0400	3949.1852

4-hydroxypyrimidin-2(*1H*)-one + 2 H_2O

Cartesian coordinates

C	2.563583	-0.744205	0.022223
C	1.022940	1.122458	-0.035286
C	0.225582	-1.067162	0.022550
C	1.544315	-1.623004	0.041771
H	3.601680	-1.043217	0.032327
H	1.693561	-2.688378	0.065948
O	0.872104	2.323722	-0.080815
N	2.316596	0.584192	-0.016025
H	3.064695	1.255604	-0.037648
N	-0.008752	0.221624	0.000595
O	-0.764198	-1.919438	0.026050
H	-1.654972	-1.469575	-0.042921
O	-3.171487	-0.878802	-0.207233
H	-3.759840	-1.113019	0.510308
H	-3.076349	0.097677	-0.159885
O	-2.459260	1.657901	0.211403
H	-1.546597	1.311387	0.212260
H	-2.432882	2.413229	-0.375172

Vibrational frequencies

42.2821	64.2174	89.6387
156.7310	161.2455	212.3719
219.3582	264.7344	289.0977
344.9786	378.3130	430.5089
436.8195	487.0963	550.6399
585.9616	593.5341	644.3757

705.9389 749.6534 796.3332
810.9976 827.8369 955.5014
987.9810 999.8533 1027.7507
1041.4608 1126.5106 1225.2977
1285.2873 1365.7776 1411.7484
1503.7821 1556.5929 1623.7649
1662.5599 1694.4331 1714.8041
1818.1189 3098.7342 3228.2530
3272.5218 3447.7528 3579.3829
3669.1218 3940.1345 3947.6030

ts3f + 2 H_2O
Cartesian coordinates

C	2.421664	-0.990026	0.009121
C	1.154284	1.068933	-0.014833
C	0.031200	-1.031245	0.016031
C	1.298922	-1.725057	0.020680
H	3.411159	-1.424339	0.009614
H	1.313733	-2.801359	0.028868
O	1.158872	2.282329	-0.051292
N	2.360104	0.365187	-0.008554
H	3.190717	0.929898	-0.029470
N	0.016224	0.313541	0.019657
O	-1.036504	-1.702214	0.007149
H	-2.212078	-1.102650	-0.093532
O	-3.176087	-0.564006	-0.171680
H	-3.735744	-0.840025	0.555233
H	-2.817539	0.555110	-0.026392
O	-2.172264	1.566380	0.176751
H	-1.186177	1.110354	0.120083
H	-2.226919	2.226373	-0.515542

Vibrational frequencies
-1144.2824 51.6318 76.9828
122.6817 163.2683 200.6174
316.6602 356.0217 418.8529
436.7222 502.1208 526.2997
571.0664 605.4303 612.6015
621.2270 630.1374 703.7668
723.0286 754.0341 804.9908
811.7594 840.2435 997.4765
1015.5679 1042.9163 1121.3254
1161.5664 1228.3705 1299.0035
1322.6705 1401.2022 1436.5866
1536.7456 1555.6629 1561.3553
1613.7133 1684.1236 1689.0109
1743.9805 1832.0603 1853.4324
1955.7910 3223.1726 3267.6771
3680.2916 3921.4381 3923.0419

uracil + 2 H_2O
Cartesian coordinates

C	-2.468897	-1.050512	0.013451
C	-1.298478	1.070191	0.022403
C	-0.060641	-1.059838	-0.045700
C	-1.332539	-1.758148	-0.028374
H	-3.444822	-1.513661	0.031314
H	-1.327394	-2.834311	-0.045146
O	-1.319914	2.275278	0.057272
N	-2.460816	0.312356	0.039460
H	-3.314213	0.840680	0.079142
N	-0.146536	0.319422	-0.034189
O	1.021444	-1.627754	-0.068110
H	2.703095	-1.070940	0.163070
O	3.573354	-0.636316	0.233395
H	4.090114	-0.989726	-0.489995
H	2.914691	0.982005	-0.040558
O	2.279859	1.705368	-0.210192
H	0.733539	0.861821	-0.077865
H	2.421835	2.358928	0.473537

Vibrational frequencies

30.7205	61.5914	79.5212
164.2479	170.3339	174.9003
189.4649	248.3526	258.3236
329.0539	381.5921	414.0862
422.2431	464.3457	541.3969
564.3346	575.7177	591.0321
717.0619	747.1474	785.5684
791.8392	836.7121	907.5169
980.8938	1000.9711	1005.3841
1016.4316	1113.2077	1230.0259
1271.3862	1412.8498	1445.0493
1520.8788	1548.3833	1658.9882
1682.0597	1707.1923	1779.0686
1852.1841	3179.0384	3226.8772
3271.6349	3520.5677	3602.0081
3685.3361	3946.3230	3948.9905

4-hydroxypyrimidin-2(*1H*)-one + 3 H_2O

Cartesian coordinates

C	3.001074	-0.464112	0.365524
C	1.263602	1.156510	-0.088580
C	0.775297	-1.123628	-0.063620
C	2.127909	-1.480053	0.238978
H	4.047105	-0.608497	0.593470
H	2.411986	-2.511145	0.357454
O	0.961144	2.325640	-0.214878
N	2.587176	0.813624	0.207428
H	3.224247	1.585927	0.300424
N	0.381211	0.118093	-0.218425
O	-0.073398	-2.104795	-0.186162
H	-1.002197	-1.780423	-0.385239
O	-2.536395	-1.400287	-0.700659

H	-2.566778	-0.712333	-1.369870
H	-2.940888	-0.972684	0.082415
O	-3.441939	0.242255	1.287263
H	-4.370712	0.470600	1.272797
H	-2.989766	0.931454	0.761731
O	-2.004836	1.573510	-0.581076
H	-1.216064	1.000616	-0.491742
H	-1.619548	2.451583	-0.594168

Vibrational frequencies

31.4062	43.9685	81.4849
87.6700	120.2911	162.3081
174.1245	208.0656	216.5322
253.7563	279.5649	299.0900
352.8598	388.7859	429.6191
437.5271	444.1545	501.1213
551.1961	554.8674	585.2318
594.6994	642.5421	749.9371
786.1022	795.9969	798.3621
823.8649	838.3150	916.8548
990.1133	1000.2490	1041.4095
1126.7886	1134.7825	1225.5817
1289.2148	1362.9757	1406.3953
1497.8043	1556.6097	1621.7094
1673.2287	1698.6206	1715.6894
1724.3730	1811.9738	3040.5422
3229.3690	3273.1061	3467.4350
3514.4075	3572.9965	3668.7148
3896.2327	3915.6339	3946.9034

ts3f + 3 H_2O

Cartesian coordinates

C	2.942454	-0.584108	0.242051
C	1.252789	1.114737	-0.021913
C	0.646480	-1.173571	-0.110803
C	2.030442	-1.555716	0.096435
H	3.992726	-0.775959	0.408817
H	2.290178	-2.599740	0.141791
O	0.983508	2.311867	-0.042102
N	2.570313	0.722716	0.191732
H	3.234699	1.465932	0.313671
N	0.332473	0.133513	-0.198319
O	-0.233017	-2.062668	-0.200353
H	-1.603792	-1.736934	-0.147759
O	-2.650570	-1.571282	-0.127317
H	-2.945723	-1.640196	-1.035822
H	-3.002358	-0.458846	0.407764
O	-3.226405	0.563534	0.837768
H	-4.149757	0.788249	0.718429
H	-2.570492	1.223409	0.220072
O	-1.703989	1.699049	-0.628496
H	-0.996062	0.962328	-0.585500

H -1.158115 2.446101 -0.345984

Vibrational frequencies
-760.7394 41.9911 44.5583
81.2964 110.0092 125.3884
168.3559 201.1283 275.7073
317.2413 389.5925 421.2427
460.2137 483.0594 531.0209
569.1471 581.5245 594.1081
605.0387 622.5886 642.9873
645.5779 727.0156 754.2327
803.3780 807.2022 817.3615
844.8628 994.2872 1004.5176
1048.6857 1100.6563 1118.9223
1219.8102 1229.9491 1286.2288
1330.7271 1400.9627 1428.0110
1483.5187 1543.0198 1588.2862
1634.2239 1701.7153 1705.8505
1732.8335 1754.1982 1791.6061
1869.1043 2194.8291 2738.7191
3222.1010 3263.5798 3682.1028
3781.6007 3925.2787 3927.6210

uracil + 3 H_2O
Cartesian coordinates
C -2.963405 0.462892 0.398656
C -1.247824 -1.166418 -0.093681
C -0.745092 1.249176 -0.120731
C -2.131508 1.498445 0.230500
H -4.003133 0.586737 0.664101
H -2.454582 2.517877 0.352723
O -0.895223 -2.317525 -0.225446
N -2.544180 -0.828019 0.244671
H -3.171760 -1.601419 0.375840
N -0.415969 -0.088331 -0.265426
O 0.089331 2.122457 -0.285377
H 1.883274 1.803756 -0.419040
O 2.793914 1.463753 -0.465023
H 2.784051 0.852320 -1.204578
H 3.098410 0.325482 0.886862
O 3.151732 -0.503184 1.403061
H 4.076721 -0.616267 1.617765
H 2.428862 -1.388433 -0.004413
O 1.947266 -1.483379 -0.847123
H 0.549211 -0.348843 -0.511272
H 1.360812 -2.238308 -0.741899

Vibrational frequencies
24.2321 46.0130 67.4423
78.5179 104.5011 159.5335
172.2833 176.9053 194.1726
241.7413 254.7420 270.7164

374.1446 403.4575 414.8338
420.2027 471.0391 476.1474
534.0023 551.6816 566.3018
581.4494 589.8470 727.9885
747.7991 772.9455 791.8331
797.2718 839.0765 896.5589
990.2252 1002.0992 1005.3914
1019.6444 1110.7243 1231.2019
1275.0444 1416.1640 1449.2371
1507.4670 1538.8004 1660.9826
1679.7771 1694.7781 1708.8178
1783.7574 1836.5764 3229.9322
3272.1039 3278.6707 3510.7804
3600.6804 3638.8701 3683.6297
3862.8542 3905.3388 3949.5048

4-hydroxypyrimidin-2(*1H*)-one + 4 H_2O
Cartesian coordinates
C -3.333560 -0.615088 -0.641766
C -1.802813 1.102652 0.102936
C -1.135411 -1.136388 0.052165
C -2.408685 -1.570733 -0.439062
H -4.327275 -0.823657 -1.010613
H -2.596244 -2.612946 -0.630169
O -1.611489 2.279212 0.331737
N -3.045432 0.680794 -0.380561
H -3.726348 1.407277 -0.519548
N -0.861997 0.126718 0.290711
O -0.243175 -2.056918 0.261157
H 0.624304 -1.688256 0.630952
O 2.015907 -1.253431 1.224011
H 1.979141 -0.324955 1.486061
H 2.709439 -1.288777 0.533071
O 3.865788 -1.089549 -0.774965
H 4.779884 -1.121362 -0.495730
H 2.485686 1.610565 -0.435059
O 1.420974 1.507772 0.983140
H 0.612630 1.015174 0.703334
H 1.071984 2.323134 1.345896
O 3.105033 1.498529 -1.182595
H 3.694025 -0.159252 -1.022660
H 3.703293 2.242897 -1.142094

Vibrational frequencies
16.2063 22.0029 42.3203
60.6488 78.0437 103.9895
161.8701 167.0132 180.5976
201.6903 208.8866 218.4070
251.7130 266.5954 271.8662
299.0153 339.7552 399.5404
430.1202 447.3248 470.1805
543.8821 546.3450 559.4643

591.8776 597.7787 639.6419
679.6767 719.6252 750.5458
797.3130 807.0006 828.6329
830.1911 891.7693 937.0759
994.6543 999.8391 1044.4431
1125.7312 1131.3793 1226.2712
1295.3049 1378.3523 1420.0029
1512.1474 1564.5522 1626.3935
1679.5071 1690.6508 1701.5410
1716.0757 1718.7666 1813.2856
2877.5578 3228.8732 3272.5547
3336.2444 3472.3561 3541.0298
3574.1172 3670.3834 3785.5542
3924.1377 3949.0814 3956.0325

ts3f + 4 H_2O
Cartesian coordinates
C -3.328384 -0.348347 -0.527405
C -1.539073 1.139542 0.099276
C -1.157552 -1.196675 0.043221
C -2.531919 -1.414789 -0.375184
H -4.362862 -0.416811 -0.832345
H -2.877505 -2.419883 -0.548908
O -1.183677 2.305177 0.283568
N -2.851198 0.904528 -0.295736
H -3.429032 1.718544 -0.403934
N -0.729115 0.068073 0.257048
O -0.393876 -2.172370 0.202099
H 0.978703 -1.890534 0.663137
O 1.947675 -1.697204 0.971049
H 1.873618 -1.041248 1.666176
H 2.734795 -1.282729 -0.082264
O 3.334575 -0.928091 -0.896175
H 4.197206 -1.340939 -0.858529
H 2.377257 1.572158 -0.090895
O 1.368768 1.538846 0.855732
H 0.737452 0.776652 0.659649
H 0.709112 2.251338 0.776340
O 3.195902 1.457105 -0.773621
H 3.352579 0.261549 -0.863368
H 3.957508 1.897597 -0.394894

Vibrational frequencies
-706.0590 26.2853 35.2617
61.3996 77.0220 85.9610
97.6066 145.2025 166.4286
201.5174 249.7732 281.5240
393.1781 410.2990 420.6371
435.0069 464.2286 496.7791
561.6325 583.6895 588.4871
597.5547 606.6032 617.9525
626.6218 641.4446 683.8182

707.4773 753.4576 803.3453
807.3054 844.7293 855.0113
992.6362 1000.3084 1044.7112
1064.2456 1115.7374 1118.1052
1203.8990 1221.7523 1333.4626
1345.3315 1400.9117 1415.7548
1436.5703 1534.2706 1599.5794
1677.0615 1692.4482 1708.8030
1734.4758 1738.3385 1778.5619
1850.5029 2001.7781 2047.7518
2540.3612 2971.6102 3220.8468
3261.4641 3658.0529 3684.3681
3913.0518 3924.6395 3936.5009

uracil + 4 H_2O
Cartesian coordinates
C -3.435088 -0.433401 -0.546682
C -1.732381 1.168312 0.066566
C -1.235799 -1.250600 0.006632
C -2.610774 -1.478518 -0.401884
H -4.467780 -0.542343 -0.844197
H -2.934794 -2.490565 -0.573304
O -1.384426 2.307664 0.284203
N -3.019785 0.848933 -0.320753
H -3.648202 1.626805 -0.416274
N -0.901158 0.083147 0.182055
O -0.414601 -2.130157 0.193516
H 1.282500 -1.789265 0.889235
O 2.141340 -1.449246 1.190136
H 1.962124 -0.546528 1.477051
H 3.179929 -1.288074 -0.187751
O 3.750853 -1.054574 -0.951996
H 4.600090 -1.454549 -0.771338
H 2.105573 1.546111 0.313223
O 1.453717 1.361131 1.024130
H 0.061706 0.326582 0.444160
H 0.868520 2.122323 1.065315
O 3.309739 1.614717 -0.926049
H 3.558604 0.671559 -1.031687
H 4.109611 2.062358 -0.652864

Vibrational frequencies
18.7519 21.9699 44.8557
58.3334 75.5773 97.1866
146.8634 152.2114 166.1991
174.7589 187.8849 255.6819
263.5478 271.5098 288.0713
294.4456 407.6712 412.5293
421.7792 450.7313 484.2784
521.4566 530.3103 551.2887
565.5906 582.0444 585.7031
628.9155 704.7150 745.4921

781.4503 791.6554 798.2047
836.6542 855.0747 972.7975
999.3955 1002.1276 1005.5781
1020.4424 1109.2076 1231.0297
1275.2726 1416.2750 1448.7277
1506.9935 1536.9904 1676.4020
1683.7628 1701.3894 1708.7117
1716.0246 1788.4351 1836.4205
3229.7444 3271.3300 3303.7048
3396.1920 3466.8357 3516.9252
3659.1501 3683.5582 3819.2192
3875.879446.8939 3953.7791

2) SCRF/PCM//ωB97X-D/6-311G(d,p) for 4-hydroxypyrimidin-2(1H)-one → ts3f → uracil pathway with H_2O solvent molecules

4-hydroxypyrimidin-2(*1H*)-one + 0 H_2O
Cartesian coordinates

C	-0.017481	-1.706692	0.000000
C	-1.204907	0.396605	0.000000
C	1.104179	0.347226	0.000000
C	1.173425	-1.069036	0.000000
H	-0.115927	-2.781378	0.000000
H	2.113044	-1.593180	0.000000
O	-2.282834	0.967998	0.000000
N	-1.163753	-0.997175	0.000000
H	-2.052919	-1.470116	0.000000
N	0.000000	1.042092	0.000000
O	2.258955	1.003667	0.000000
H	2.061814	1.948316	0.000000

Vibrational frequencies

157.8929 218.8774 381.7387
430.6347 547.1941 560.8903
578.8955 587.2163 674.2082
752.9905 795.5124 814.3393
821.0479 976.8739 1017.1431
1030.7890 1127.8126 1205.1964
1248.1254 1284.6770 1377.3786
1484.3936 1511.5179 1622.1661
1699.9869 1750.3755 3246.6034
3274.1733 3648.7586 3809.5179

ts3f + 0 H_2O
Cartesian coordinates

C	-0.093732	-1.713902	0.000000
C	1.205589	0.345499	0.000000
C	-1.186387	0.338561	0.000000
C	-1.287310	-1.068707	0.000000
H	-0.019432	-2.791042	0.000000
H	-2.228009	-1.589682	0.000000
O	2.293961	0.882675	0.000000

N	1.082224	-1.049421	0.000000
H	1.947318	-1.565397	0.000000
N	0.000000	0.972718	0.000000
O	-2.067342	1.263476	0.000000
H	-0.917357	1.905127	0.000000

Vibrational frequencies

-1953.5888	175.5688	185.2630
412.3590	422.2776	540.1774
604.1794	635.4958	653.8206
721.0609	791.7325	797.6780
802.8462	1012.4336	1023.5046
1084.5583	1101.7005	1113.9043
1239.6532	1346.2676	1404.5781
1444.3505	1531.5227	1613.9858
1666.6771	1783.4528	2150.6335
3244.5020	3281.0338	3652.0440

uracil + 0 H_2O

Cartesian coordinates

C	0.053272	-1.695214	0.000000
C	-1.221361	0.350612	0.000000
C	1.262126	0.388879	0.000000
C	1.233280	-1.057625	0.000000
H	-0.028464	-2.771387	0.000000
H	2.164918	-1.597069	0.000000
O	-2.277857	0.947018	0.000000
N	-1.132763	-1.020671	0.000000
H	-2.004656	-1.522685	0.000000
N	0.000000	0.980999	0.000000
O	2.260464	1.085395	0.000000
H	-0.027218	1.989617	0.000000

Vibrational frequencies

164.5606	176.1562	394.1297
411.9321	531.2402	557.3898
573.3356	593.6920	678.7150
745.0783	789.8196	789.8452
834.6543	995.7943	1006.1613
1015.0807	1112.5058	1230.1217
1251.7986	1405.9822	1434.5395
1446.1656	1530.1363	1699.5412
1752.3904	1798.9403	3244.4475
3269.2308	3634.3237	3667.4112

4-hydroxypyrimidin-2(*1H*)-one + 1 H_2O

Cartesian coordinates

C	-1.959579	-1.062548	0.018735
C	-0.866294	1.088551	-0.005920
C	0.380539	-0.873004	-0.008547
C	-0.771259	-1.703143	0.009237
H	-2.909702	-1.574413	0.032309

H	-0.691453	-2.776174	0.014632
O	-0.981158	2.303154	-0.011158
N	-2.003857	0.285553	0.011595
H	-2.889666	0.764539	0.018624
N	0.335726	0.439905	-0.016529
O	1.554730	-1.472085	-0.018928
H	2.267545	-0.788378	-0.024086
O	3.111520	0.736695	-0.072765
H	3.514400	0.965187	0.767219
H	2.204622	1.089795	-0.032377

Vibrational frequencies

65.0061	120.1847	165.4815
203.9860	211.4979	315.0915
368.4967	420.1873	438.5609
548.9868	578.0889	592.0268
670.5237	712.0709	748.4643
800.1423	814.0278	825.0712
905.2174	993.0297	1017.0676
1046.8266	1129.1035	1231.8497
1286.6502	1345.5705	1408.1330
1508.4515	1515.5385	1622.4954
1648.7884	1697.6875	1751.8019
3243.3590	3272.9509	3323.3921
3605.4017	3658.2492	3911.3989

ts3f + 1 H_2O

Cartesian coordinates

C	-1.813401	-1.192954	0.018075
C	-0.897624	1.039841	-0.006216
C	0.532114	-0.867481	-0.008424
C	-0.587322	-1.753042	0.009619
H	-2.724670	-1.771564	0.031117
H	-0.443006	-2.819547	0.015369
O	-1.090053	2.243385	-0.011101
N	-1.964747	0.151655	0.010724
H	-2.884465	0.560206	0.017106
N	0.337809	0.466892	-0.016804
O	1.731767	-1.301466	-0.018981
H	2.454270	-0.281789	-0.023303
O	2.719743	0.866189	-0.071037
H	3.117641	1.148625	0.756399
H	1.574535	1.011187	-0.023493

Vibrational frequencies

-1552.9016	96.6485	180.4195
197.1113	267.3425	434.5819
439.4285	538.8131	555.5196
571.3077	618.1157	630.4395
652.5767	685.9761	755.0658
805.6122	819.0719	836.6015
847.0152	1018.5222	1030.3869

1077.5546 1124.2836 1237.4818
1325.1768 1371.4303 1404.9656
1459.9228 1504.4748 1544.8768
1600.6070 1659.5698 1701.6338
1769.2797 2002.2262 3240.8359
3270.5348 3663.6165 3885.3538

uracil + 1 H_2O
Cartesian coordinates
C -1.981939 -1.020984 0.025666
C -0.866611 1.114769 -0.008380
C 0.419775 -0.994607 -0.013681
C -0.830997 -1.712057 0.012401
H -2.949476 -1.498911 0.044928
H -0.817255 -2.788315 0.020381
O -0.892584 2.327496 -0.016289
N -2.003564 0.341130 0.015512
H -2.879390 0.836602 0.026197
N 0.297991 0.386530 -0.022586
O 1.531281 -1.513310 -0.029310
H 2.871965 -0.184346 -0.039609
O 3.183251 0.735963 -0.063882
H 3.526189 0.904221 0.815254
H 1.170018 0.913217 -0.037816

Vibrational frequencies
59.5441 94.7220 168.2090
172.4866 179.3931 275.9475
351.2651 406.2657 422.8369
538.1429 566.3837 578.9292
614.5614 702.8547 746.7610
784.8350 796.6007 822.2383
845.8012 1006.0719 1018.1267
1019.2627 1115.9826 1239.1464
1264.4468 1417.0843 1452.4606
1464.0642 1537.7288 1647.5802
1696.7368 1730.6886 1794.9489
3244.1559 3270.9274 3451.9496
3635.3093 3668.4546 919.9182

4-hydroxypyrimidin-2(*1H*)-one + 2 H_2O
Cartesian coordinates
C -2.549875 -0.797838 0.005836
C -1.072704 1.105032 -0.019500
C -0.208037 -1.054749 0.011624
C -1.502313 -1.646936 0.019790
H -3.579196 -1.122573 0.009817
H -1.625235 -2.715823 0.036250
O -0.951313 2.320074 -0.032524
N -2.340061 0.535298 -0.013330
H -3.118171 1.173955 -0.022013
N -0.009242 0.245285 -0.009768

O	0.812275	-1.875814	0.028907
H	1.694111	-1.407336	0.021954
O	3.240793	-0.853958	0.042050
H	3.694821	-1.066758	-0.775192
H	3.127659	0.120517	0.037681
O	2.427630	1.709450	-0.037712
H	1.529620	1.317935	-0.039857
H	2.484010	2.204927	0.780780

Vibrational frequencies

25.9775	63.1481	93.9024
164.8235	168.9879	215.9446
217.1203	263.2878	279.1191
358.1203	397.1830	434.7496
445.1719	494.0359	554.2057
583.7711	593.6951	661.8405
698.8640	750.0732	802.1263
813.7106	826.5952	943.7490
987.6906	996.5665	1017.8960
1050.2960	1130.5547	1227.4485
1287.9499	1344.2514	1405.6233
1494.8642	1528.6019	1614.0929
1649.1296	1665.2487	1694.4638
1747.7557	3104.6554	3242.6414
3272.4962	3430.0764	3504.2055
3657.5970	3914.3293	3919.2428

ts3f + 2 H_2O

Cartesian coordinates

C	2.437997	-0.985607	0.000721
C	1.170365	1.060535	0.020951
C	0.046848	-1.031237	-0.022555
C	1.313719	-1.720739	-0.022796
H	3.428738	-1.414516	0.003217
H	1.337771	-2.797206	-0.040609
O	1.174099	2.286054	0.035409
N	2.372187	0.368475	0.022596
H	3.211040	0.923279	0.038106
N	0.030159	0.318782	0.001798
O	-1.024022	-1.696984	-0.046278
H	-2.292225	-1.093102	-0.012255
O	-3.224077	-0.581266	-0.010882
H	-3.690425	-0.794603	0.801202
H	-2.855583	0.536301	0.000134
O	-2.202886	1.575762	0.018373
H	-1.233394	1.141003	-0.002423
H	-2.320819	2.081800	-0.789026

Vibrational frequencies

-886.9534	46.4234	65.0092
122.1322	167.2090	203.3887
282.6682	336.2132	424.2561

451.6974 489.2826 531.2995
571.5542 598.7312 608.1423
618.9445 626.3459 683.4300
733.5481 753.4976 809.5107
809.9775 838.0915 1011.3189
1013.1768 1041.1575 1125.8355
1138.9270 1229.5084 1245.5653
1322.3662 1401.1554 1426.6852
1522.2887 1549.3497 1557.1229
1594.9052 1663.9159 1691.0889
1726.8799 1802.1493 2083.4801
2103.6119 3237.3090 3262.4189
3662.8376 3888.9983 3892.9842

uracil + 2 H_2O
Cartesian coordinates

C	2.485109	-1.007655	0.019046
C	1.276104	1.074975	0.043285
C	0.084673	-1.074484	-0.071024
C	1.363401	-1.741698	-0.047572
H	3.471074	-1.445957	0.040875
H	1.391886	-2.817136	-0.082599
O	1.254555	2.288042	0.080262
N	2.446648	0.352398	0.063759
H	3.298266	0.886128	0.113461
N	0.139556	0.304879	-0.023077
O	-0.994825	-1.657890	-0.130429
H	-2.657404	-1.093966	0.032360
O	-3.544826	-0.694906	0.118879
H	-3.827768	-0.900138	1.011228
H	-2.915535	0.960753	-0.001716
O	-2.326291	1.737384	-0.076169
H	-0.746733	0.829746	-0.048143
H	-2.481839	2.091767	-0.953000

Vibrational frequencies
25.6871 60.2179 83.5843
160.6270 175.3531 177.0120
189.9588 243.9487 269.9476
323.6435 384.9410 413.0325
428.3245 471.7326 541.6676
566.1386 578.4057 614.6892
680.2610 747.2354 790.1384
798.4183 834.6042 906.0209
942.4570 1004.7595 1019.6184
1027.3810 1118.7173 1236.0321
1269.5256 1419.5213 1452.7029
1502.9136 1543.5558 1650.8414
1657.7015 1697.5248 1724.3136
1794.0377 3237.2940 3244.8701
3270.7212 3493.8155 3557.3721
3661.9444 3918.5245 3921.3057

4-hydroxypyrimidin-2(*1H*)-one + 3 H_2O
Cartesian coordinates

C	3.031948	-0.402350	0.285466
C	1.222352	1.152135	-0.036681
C	0.821572	-1.136988	-0.057457
C	2.190808	-1.450237	0.168879
H	4.091705	-0.506549	0.460710
H	2.524847	-2.470251	0.246157
O	0.863238	2.320901	-0.109820
N	2.560254	0.858870	0.187147
H	3.182576	1.645044	0.278795
N	0.370028	0.093142	-0.165541
O	-0.009606	-2.143332	-0.157765
H	-0.956445	-1.844304	-0.265642
O	-2.572844	-1.658220	-0.384459
H	-2.858018	-1.443404	-1.274152
H	-2.955960	-0.959409	0.188547
O	-3.492456	0.434603	1.097054
H	-4.420847	0.613766	0.940831
H	-3.002249	1.058292	0.521796
O	-1.923409	1.661473	-0.725250
H	-1.275992	0.933395	-0.664996
H	-1.361055	2.410576	-0.502617

Vibrational frequencies

31.7138	32.6728	72.7441
80.3220	93.5905	166.1398
170.7867	199.6831	218.3928
250.7796	276.7957	292.6487
331.1511	365.3303	414.0614
431.8051	440.9405	444.1025
502.7588	556.6044	583.0870
595.1347	669.4411	746.5554
753.1932	770.3758	803.2434
816.0981	829.3446	954.6981
992.3529	1018.1142	1044.9673
1058.1388	1129.7128	1227.3598
1291.8260	1335.4411	1400.7860
1489.5491	1527.1633	1613.7266
1651.2691	1670.2924	1686.5509
1704.2481	1742.4861	3104.2009
3243.4345	3272.4763	3417.6702
3492.3739	3572.6707	3654.5844
3851.7070	3916.9375	3920.3049

ts3f + 3 H_2O
Cartesian coordinates

C	2.979227	-0.710815	0.199337
C	1.402443	1.096069	0.014090
C	0.640618	-1.140481	-0.112350
C	1.998366	-1.616103	0.054271

H	4.018141	-0.972498	0.334459
H	2.197777	-2.674713	0.067295
O	1.212277	2.313413	0.010845
N	2.692537	0.615729	0.185585
H	3.420020	1.300727	0.297762
N	0.408055	0.189062	-0.144256
O	-0.298714	-1.966797	-0.222889
H	-1.771690	-1.670196	-0.118448
O	-2.789086	-1.596964	-0.025086
H	-3.162969	-1.813554	-0.881851
H	-3.190586	-0.411461	0.369754
O	-3.440306	0.621335	0.693718
H	-4.332377	0.849207	0.417083
H	-2.744635	1.226498	0.178266
O	-1.687928	1.764740	-0.597270
H	-0.937998	1.095521	-0.487083
H	-1.293693	2.579092	-0.273174

Vibrational frequencies

-261.8822	28.6300	34.7013
57.9338	92.1984	121.4174
163.1193	201.3915	224.7590
293.9858	386.3198	422.7035
445.9972	452.0075	483.2557
491.8759	557.3746	575.2619
593.5391	607.2465	615.2178
620.5134	753.1513	768.9185
805.6946	809.2906	839.2097
981.5484	1001.0834	1007.4698
1041.0475	1062.8052	1105.3055
1123.9728	1211.4722	1228.0815
1323.9123	1397.0269	1417.9453
1422.9186	1538.1899	1572.3112
1681.0084	1683.5475	1697.1773
1715.3375	1760.2539	1814.2145
2171.1828	2640.7034	2872.9871
3232.1774	3257.3861	3672.1925
3877.3625	3881.9792	3902.3384

uracil + 3 H_2O

Cartesian coordinates

C	-2.956940	0.485513	0.406037
C	-1.263339	-1.155084	-0.061365
C	-0.752566	1.250587	-0.165422
C	-2.123173	1.516145	0.195075
H	-3.991288	0.617407	0.683931
H	-2.449125	2.536967	0.296162
O	-0.899265	-2.313081	-0.160873
N	-2.543797	-0.807580	0.285976
H	-3.182345	-1.566162	0.458243
N	-0.430596	-0.087514	-0.287304
O	0.098668	2.113197	-0.359427

H	1.843432	1.831845	-0.295781
O	2.802275	1.668038	-0.208686
H	3.097304	1.444229	-1.092862
H	3.130421	0.249000	0.811611
O	3.223702	-0.619968	1.250645
H	4.166233	-0.788916	1.283529
H	2.392013	-1.472940	-0.110810
O	1.861646	-1.665409	-0.906145
H	0.519065	-0.350007	-0.569804
H	1.174946	-2.280955	-0.624982

Vibrational frequencies

25.9924	29.9302	51.9916
73.5440	88.7899	158.0562
174.6020	181.6471	185.2965
232.0799	252.7399	275.7589
281.7734	386.6464	410.4732
425.2179	458.3919	481.7379
541.3488	558.9759	577.1805
582.3512	613.3797	718.2305
746.2914	776.7478	788.3211
802.1561	834.4871	847.1906
945.9328	1007.0318	1018.8537
1027.5113	1116.0972	1238.5299
1272.5957	1418.6080	1454.6734
1484.6995	1538.6571	1645.5364
1657.7982	1672.9750	1697.0753
1721.7622	1783.8606	3244.3423
3271.3055	3347.5444	3482.3610
3546.5896	3583.0754	3661.4284
3809.8842	3917.9153	3922.6605

4-hydroxypyrimidin-2(*1H*)-one + 4 H_2O

Cartesian coordinates

C	-3.368806	-0.459361	-0.590424
C	-1.721565	1.159301	0.095802
C	-1.198686	-1.104680	0.053528
C	-2.496439	-1.470359	-0.400390
H	-4.381607	-0.604777	-0.933685
H	-2.755482	-2.498948	-0.581520
O	-1.443624	2.331205	0.297006
N	-2.991929	0.814239	-0.350659
H	-3.639628	1.572381	-0.490588
N	-0.836697	0.135149	0.289384
O	-0.343929	-2.083917	0.234693
H	0.552859	-1.770207	0.517662
O	2.167792	-1.534527	0.939584
H	2.578315	-2.251023	1.425828
H	2.723656	-1.369280	0.140994
O	3.530241	-0.818397	-1.250712
H	4.476957	-0.951980	-1.184451
H	2.459777	1.688551	-0.039262

O	1.606832	1.171523	1.402777
H	0.724589	0.940273	1.054743
H	1.998451	0.296104	1.530207
O	2.942047	1.814889	-0.885131
H	3.397416	0.152628	-1.199858
H	3.703191	2.354947	-0.667982

Vibrational frequencies

13.3943	21.9225	32.6589
65.2554	70.1452	98.4219
155.9816	167.7328	185.6535
208.7828	219.8510	244.9776
262.1483	267.0204	281.9455
313.7082	338.3882	401.2380
421.1671	439.0579	458.0406
497.7117	553.4884	557.3069
583.5080	593.6188	621.8915
665.3431	748.5808	764.1894
777.3344	802.2150	813.7890
826.2248	827.5113	961.8877
990.5766	1000.7758	1018.2100
1046.8447	1130.6127	1226.1220
1285.4851	1319.4985	1397.1624
1487.5949	1526.6843	1612.7313
1663.7205	1666.7039	1675.6678
1686.3794	1697.0647	1751.4648
3236.4376	3243.5947	3272.4862
3334.7774	3409.2785	3478.7218
3571.0595	3651.8364	3747.1064
3917.7871	3921.1561	3922.0337

ts3f + 4 H_2O

Cartesian coordinates

C	-3.311193	-0.655574	-0.594480
C	-1.835852	1.110875	0.118626
C	-1.053800	-1.120134	0.069225
C	-2.346867	-1.570438	-0.406250
H	-4.303256	-0.896438	-0.946947
H	-2.512447	-2.617156	-0.600700
O	-1.691953	2.314934	0.327555
N	-3.066739	0.654415	-0.340647
H	-3.782284	1.347051	-0.478207
N	-0.857756	0.194258	0.311059
O	-0.134569	-1.957673	0.249091
H	1.304326	-1.646501	0.676054
O	2.275698	-1.468548	0.915754
H	2.598032	-2.222095	1.411904
H	3.072230	-1.056902	-0.291388
O	3.522675	-0.614798	-1.102088
H	4.472161	-0.756350	-1.045478
H	2.282514	1.627903	-0.045876
O	1.480687	1.236190	1.229075

H	0.594811	0.895985	0.908949
H	1.924306	0.428274	1.518155
O	2.834199	1.684051	-0.897563
H	3.271868	0.497324	-1.046275
H	3.541579	2.316566	-0.750403

Vibrational frequencies

-333.7031	12.1802	28.2126
54.3248	66.0505	74.6970
124.7790	159.7938	170.6470
203.2978	214.8823	243.3768
348.5965	365.0944	418.7618
424.4807	447.0976	463.5357
469.3264	549.5957	570.5400
577.5670	592.3865	605.8357
610.2381	667.1080	688.0027
752.7278	786.0623	802.9773
809.8999	836.8007	898.2205
979.6018	995.5892	1001.4859
1005.6665	1043.9321	1062.6647
1123.2706	1167.1059	1225.5560
1321.7369	1370.9231	1392.6590
1415.5278	1535.6506	1565.5159
1668.9446	1680.8549	1695.4965
1709.1808	1734.3651	1739.1190
1845.2711	2562.2343	2779.8079
2806.9585	3069.5112	3229.8316
3255.0214	3674.7832	3779.5491
3875.1673	3892.5672	3921.1528

uracil + 4 H_2O

Cartesian coordinates

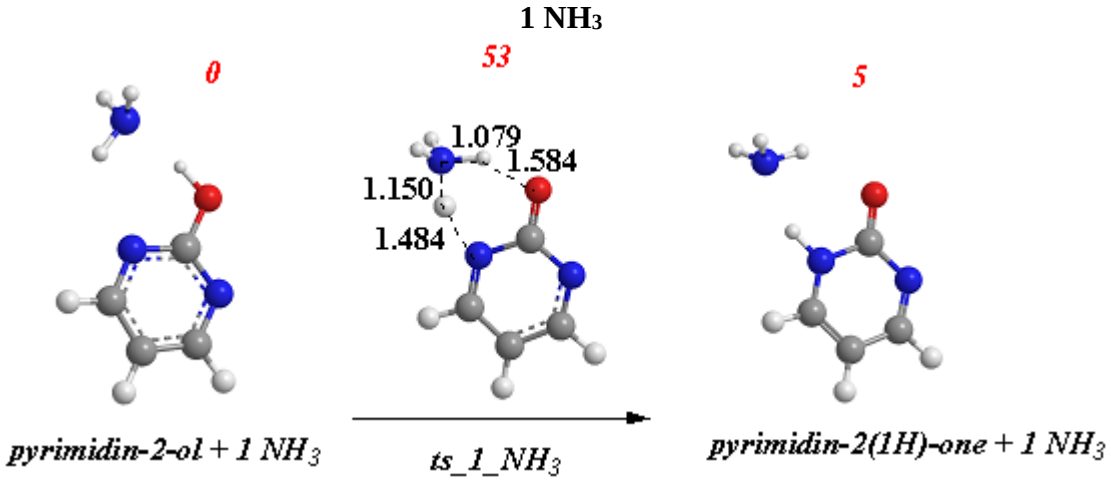
C	-3.352967	-0.648267	-0.644936
C	-1.941234	1.129331	0.159304
C	-1.098455	-1.172368	-0.003424
C	-2.389688	-1.572723	-0.504928
H	-4.339691	-0.881373	-1.015073
H	-2.554791	-2.605878	-0.757675
O	-1.764187	2.297326	0.438307
N	-3.139588	0.656950	-0.324986
H	-3.872888	1.336679	-0.436698
N	-0.969456	0.167316	0.297586
O	-0.156183	-1.946940	0.156924
H	1.447740	-1.740963	0.714778
O	2.366039	-1.537124	0.995464
H	2.634603	-2.228490	1.601229
H	3.392666	-1.038052	-0.387690
O	3.854766	-0.620928	-1.138291
H	4.785805	-0.658598	-0.914445
H	1.956588	1.496799	0.553646
O	1.493158	1.093937	1.312160
H	-0.062100	0.505156	0.662150

H	1.939936	0.242556	1.432019
O	2.864063	1.937603	-0.947722
H	3.280912	1.064271	-1.090255
H	3.587345	2.531204	-0.741012

Vibrational frequencies

13.9570	23.0919	31.6211
63.1604	72.8814	98.3734
162.6237	177.2253	182.0714
183.1305	205.1667	232.7608
243.6164	254.3803	263.9193
271.0659	290.4617	385.0557
414.3650	425.7911	475.1510
521.9054	537.3786	546.4616
567.8764	582.9026	621.2651
670.9496	680.0879	747.3009
756.2143	792.6343	799.9127
833.0950	834.9424	866.8355
984.8483	1005.8024	1018.9868
1029.9852	1119.3607	1238.2608
1272.0414	1418.0719	1453.7009
1511.3696	1548.0397	1644.1689
1666.0911	1670.9524	1695.8674
1698.2536	1723.7420	1794.2464
3163.1835	3242.9246	3270.7073
3424.8043	3488.6689	3570.5742
3590.0660	3671.6316	3707.1285
3920.4979	3922.5783	3930.5662

3) ωB97X-D/6-311G(d,p) for pyrimidin-2-ol → ts3c → pyrimidin-2(*1H*)-one pathway with NH_3 and CH_3OH solvent molecules



pyrimidin-2-ol + 1 NH_3

Cartesian coordinates

C	-2.170958	0.838087	-0.000007
C	-2.173361	-0.552377	-0.000003
N	-1.067988	-1.281117	0.000002
C	0.084121	-0.602819	0.000002
N	0.209748	0.734301	-0.000003

C	-0.921975	1.433143	-0.000007
O	1.176725	-1.333769	0.000006
H	-3.084968	1.415460	-0.000011
H	-3.108354	-1.107515	-0.000003
H	-0.813945	2.514739	-0.000011
H	1.980408	-0.746882	0.000007
N	3.224855	0.477449	0.000007
H	3.808441	0.585090	0.820458
H	3.808451	0.585083	-0.820439
H	2.522897	1.213541	0.000000

Vibrational frequencies

53.9084	117.6265	140.8321
182.4550	224.8213	291.2906
423.2051	437.5575	545.3357
555.6229	610.2433	663.7294
816.0002	846.5682	908.1091
1002.4309	1016.7129	1018.0931
1043.2105	1103.7223	1109.4426
1120.9844	1248.3623	1302.1443
1409.1163	1451.4138	1517.9345
1542.0732	1642.8343	1665.5079
1682.9845	1686.8173	3170.7745
3174.2351	3200.1676	3237.0332
3500.6832	3628.5659	3658.3306

ts_1_NH_3

Cartesian coordinates

C	2.059747	0.881156	-0.000004
C	2.105674	-0.520545	-0.000030
N	1.051476	-1.301844	-0.000019
C	-0.180922	-0.707676	0.000018
N	-0.301234	0.674917	0.000030
C	0.798092	1.427133	0.000022
O	-1.222089	-1.403653	0.000040
H	2.953700	1.488239	-0.000012
H	3.069755	-1.028113	-0.000063
H	0.643628	2.503655	0.000047
H	-2.480325	-0.440970	-0.000008
N	-2.838423	0.577097	-0.000038
H	-3.365858	0.804361	-0.834266
H	-3.365912	0.804396	0.834147
H	-1.756547	0.966062	-0.000008

Vibrational frequencies

-567.0634	81.9981	153.9198
333.8524	378.9911	407.8778
446.8840	456.9489	535.4928
590.3088	616.9712	680.6984
794.1110	845.7157	875.5298
907.3930	988.7064	1008.2267
1021.7543	1079.4667	1136.9216

1198.5853	1319.4686	1396.4410
1434.9555	1506.0798	1562.1156
1579.1383	1623.1199	1644.6575
1689.4482	1698.1882	1977.6225
2666.5290	3146.3394	3167.2446
3235.2819	3567.2288	3659.8161

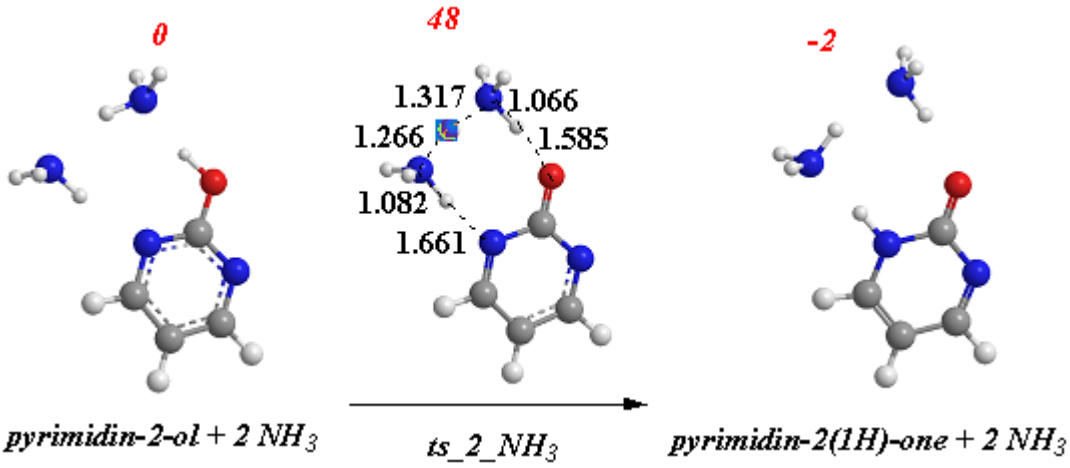
pyrimidin-2(1H)-one + 1 NH_3
Cartesian coordinates

C	-2.004432	1.030984	-0.000009
C	-2.182589	-0.376195	-0.000010
N	-1.226149	-1.259262	-0.000005
C	0.086682	-0.823988	0.000002
N	0.288665	0.567213	0.000003
C	-0.714502	1.461605	-0.000002
O	1.047125	-1.568916	0.000008
H	-2.838991	1.715742	-0.000013
H	-3.195321	-0.778257	-0.000015
H	-0.428775	2.507177	-0.000001
H	2.903404	-0.398066	0.000009
N	3.135311	0.595291	0.000008
H	3.702824	0.783621	0.817659
H	3.702822	0.783621	-0.817644
H	1.281290	0.860358	0.000007

Vibrational frequencies

62.4698	126.6458	134.5138
158.5396	206.3621	316.2116
404.3186	481.1619	518.7652
520.8337	586.9730	642.7590
789.5440	823.6511	865.5230
975.1295	1006.6499	1009.8118
1047.7777	1057.0824	1135.5636
1140.4272	1179.0398	1271.8101
1407.5963	1478.5350	1537.3001
1626.0111	1667.6065	1700.3864
1709.7942	1819.1198	3148.3710
3207.6957	3211.1955	3258.3068
3470.7329	3604.6897	3649.8334

2 NH_3



pyrimidin-2-ol + 2 NH_3

Cartesian coordinates

C	-2.413307	1.102242	0.000012
C	-2.717359	-0.255550	0.000002
N	-1.798769	-1.206604	-0.000008
C	-0.520740	-0.801881	-0.000009
N	-0.112601	0.478221	-0.000001
C	-1.065425	1.407334	0.000010
O	0.372558	-1.755797	-0.000018
H	-3.178342	1.865892	0.000022
H	-3.750909	-0.594010	0.000003
H	-0.721493	2.439341	0.000017
H	1.321467	-1.416190	-0.000008
N	2.991641	-1.128889	0.000022
H	3.446998	-1.522271	0.815889
H	3.447051	-1.522324	-0.815790
H	3.155071	-0.114955	-0.000002
N	2.677320	1.839564	-0.000017
H	2.786065	2.427820	0.817140
H	2.786074	2.427819	-0.817173
H	1.725413	1.466334	-0.000021

Vibrational frequencies

22.6285	61.4632	95.5478
146.9846	170.1119	177.8770
218.7557	219.7551	250.3860
301.7157	402.6299	425.7041
425.9316	531.4469	548.7451
612.4269	639.1211	664.3962
813.5608	845.9323	911.2571
1011.1072	1018.4461	1019.0431
1104.1518	1115.4713	1125.9199
1132.4750	1213.3199	1249.1271
1302.9239	1411.9171	1446.4585
1507.2858	1556.5562	1636.8599
1658.1767	1677.4219	1687.1408
1706.4802	1719.2656	2982.9927
3158.5944	3163.4088	3237.4345

3361.5150	3429.2679	3575.0148
3591.6222	3639.5214	3649.2584

ts_2_NH_3

Cartesian coordinates

C	2.588742	0.860169	-0.000255
C	2.658303	-0.538431	-0.000019
N	1.614624	-1.333161	0.000191
C	0.366100	-0.758735	0.000170
N	0.218356	0.616130	-0.000018
C	1.311350	1.375100	-0.000228
O	-0.643557	-1.493370	0.000332
H	3.469451	1.486740	-0.000431
H	3.630212	-1.032569	0.000003
H	1.143810	2.452113	-0.000376
H	-2.193669	-1.164651	-0.000236
N	-3.193588	-0.795512	-0.000499
H	-3.677468	-1.138933	-0.822506
H	-3.678065	-1.139403	0.820960
H	-2.917802	0.492348	-0.000057
N	-2.330760	1.614044	0.000390
H	-2.520166	2.175675	-0.822556
H	-2.520138	2.174967	0.823826
H	-1.295098	1.301563	0.000250

Vibrational frequencies

-926.8101	21.1246	61.8064
96.5855	147.9872	270.2715
296.1322	301.8535	338.3057
411.0939	443.8749	542.7153
547.5081	589.3278	623.0566
639.2156	667.0896	674.0927
787.5387	838.8801	847.3008
901.4640	994.7377	1011.3482
1020.4721	1085.2282	1125.1708
1193.6785	1317.1142	1358.0844
1410.7421	1434.2763	1490.0748
1545.7418	1585.5664	1614.3190
1657.2031	1689.8836	1699.1987
1704.8112	1767.3106	1810.9064
2468.9439	2747.7161	3126.6866
3128.5534	3233.4337	3552.2855
3558.5705	3638.3774	3641.5649

pyrimidin-2(1H)-one + 2 NH_3

Cartesian coordinates

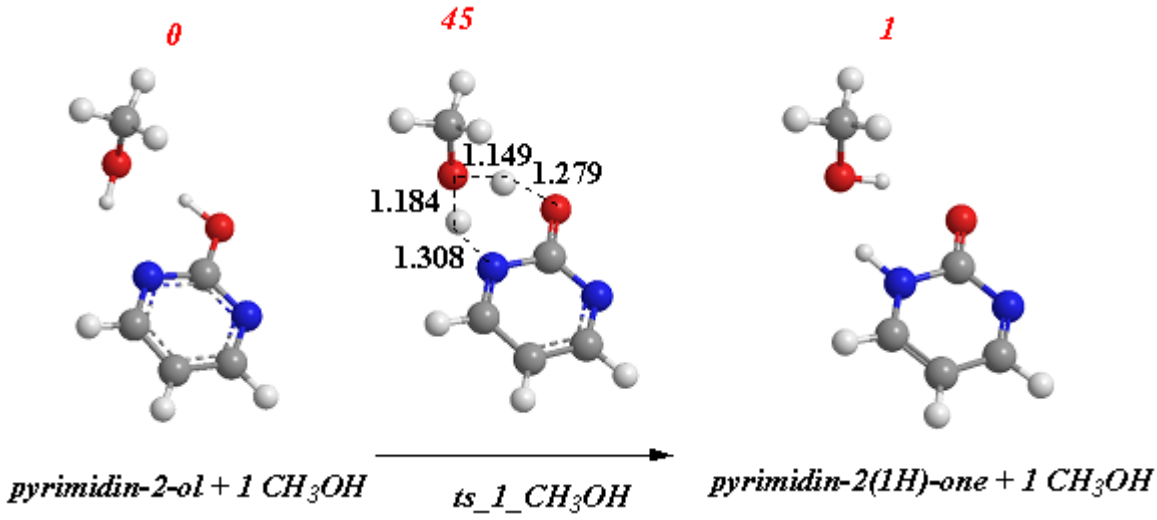
C	-2.611824	0.860218	-0.000176
C	-2.691880	-0.554203	0.000053
N	-1.673736	-1.366419	0.000189
C	-0.395136	-0.839214	0.000107
N	-0.287304	0.556804	-0.000104
C	-1.352324	1.375175	-0.000242

O	0.607731	-1.528735	0.000213
H	-3.491348	1.486303	-0.000282
H	-3.673430	-1.027266	0.000127
H	-1.133220	2.437248	-0.000409
H	2.562522	-1.224714	0.000188
N	3.516639	-0.857636	0.000162
H	3.985488	-1.237726	0.814240
H	3.985522	-1.237932	-0.813801
H	2.872018	1.010080	-0.000080
N	2.256945	1.838802	-0.000182
H	2.491325	2.393959	0.815153
H	2.491396	2.393811	-0.815597
H	0.667051	0.983407	-0.000144

Vibrational frequencies

18.3004	63.7148	73.5894
143.4762	153.1931	168.2800
214.0006	221.0679	243.4754
312.2703	407.2384	413.8076
425.6821	516.7579	526.3060
591.7992	616.6529	645.9360
789.1179	824.9940	873.1295
980.5213	1005.9025	1008.0392
1050.1175	1124.4977	1137.5166
1163.4236	1185.1996	1225.6371
1279.7851	1416.0255	1484.8713
1547.5156	1640.4502	1662.3696
1681.3682	1713.1917	1714.3324
1732.2071	1806.1072	3039.3740
3147.7396	3208.4220	3248.6796
3289.7907	3441.0604	3563.6376
3585.1395	3634.1189	3637.5695

1 CH_3OH



pyrimidin-2-ol + 1 CH_3OH

Cartesian coordinates

C	-2.423931	1.014538	0.101634

C	-2.583436	-0.356828	0.270321
N	-1.585378	-1.222208	0.173577
C	-0.387262	-0.705579	-0.100439
N	-0.113472	0.596203	-0.279214
C	-1.138601	1.439787	-0.176717
O	0.602858	-1.570646	-0.199918
H	-3.251537	1.705037	0.182401
H	-3.558808	-0.781950	0.492182
H	-0.909764	2.490849	-0.325810
H	1.434306	-1.087711	-0.407599
O	2.629089	0.190359	-0.579348
C	3.240030	0.427211	0.677770
H	3.694755	1.422672	0.720506
H	4.025605	-0.317612	0.806606
H	2.523606	0.327878	1.502435
H	1.837424	0.750392	-0.632546

Vibrational frequencies

51.6235	76.8408	109.8493
141.7117	186.3045	204.6356
220.6095	425.7915	518.4493
548.4951	609.1969	662.3267
751.4930	820.3743	844.2844
906.2633	908.2408	1021.1472
1022.8933	1027.8141	1088.2613
1108.6319	1125.3377	1140.4713
1188.5498	1252.3263	1298.7767
1407.3893	1437.9982	1460.5177
1490.2939	1504.3896	1516.6432
1521.4400	1541.1897	1652.1617
1686.1425	3018.8876	3083.6969
3139.8214	3178.6384	3188.4556
3245.8020	3432.9860	3680.2414

ts_1_CH_3OH

Cartesian coordinates

C	2.349562	1.004329	-0.085921
C	2.501773	-0.381490	-0.232962
N	1.519089	-1.253136	-0.158431
C	0.279980	-0.765705	0.078448
N	0.052873	0.582901	0.228124
C	1.069376	1.442280	0.148999
O	-0.718541	-1.539423	0.172053
H	3.186011	1.684606	-0.151993
H	3.488110	-0.800471	-0.421585
H	0.826308	2.491422	0.281288
H	-1.721629	-0.781235	0.407041
O	-2.300679	0.201022	0.546883
C	-3.104900	0.456358	-0.595160
H	-3.571066	1.438227	-0.494701
H	-3.888732	-0.300017	-0.662405
H	-2.511353	0.431890	-1.517339

H	-1.232366	0.699803	0.439947

Vibrational frequencies

-1527.2530	73.0728	123.0019
158.9358	170.3775	204.3711
381.3464	422.3343	455.1419
543.8835	603.7760	662.4781
717.5885	806.2854	842.6129
902.2881	1003.7583	1012.7584
1030.3795	1071.4030	1087.8717
1146.2572	1162.8414	1176.2701
1213.7645	1235.2664	1323.9618
1395.7251	1424.9861	1497.3465
1505.8137	1515.5110	1527.8826
1560.2134	1577.5816	1621.6155
1693.8041	1761.6224	2041.7655
3027.2589	3108.1862	3138.1059
3161.4661	3202.4394	3251.3841

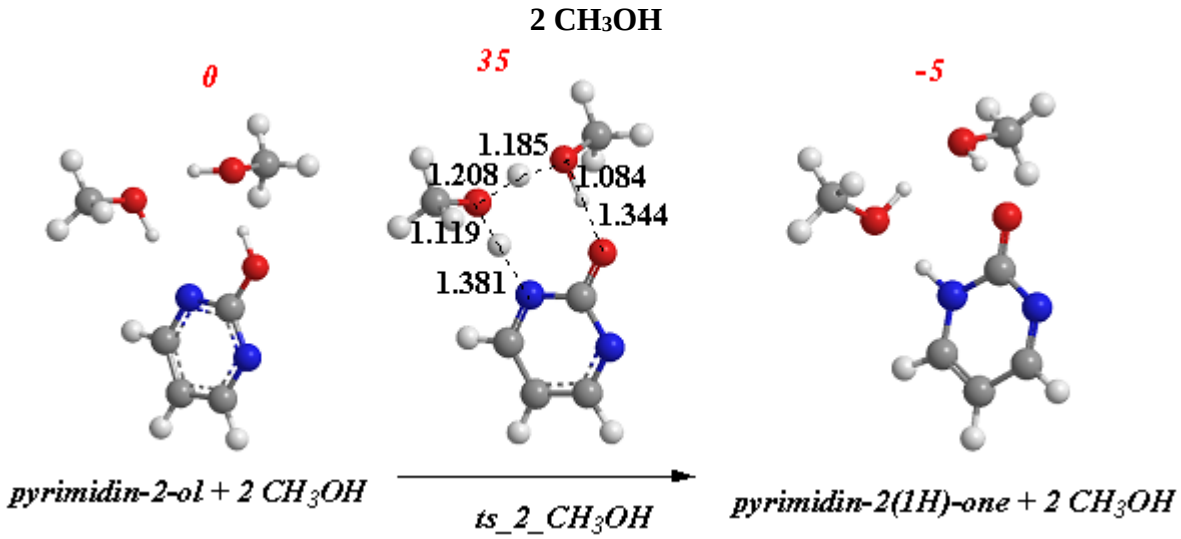
pyrimidin-2(1H)-one + 1 CH_3OH
Cartesian coordinates

C	-2.424151	1.035293	0.104127
C	-2.585583	-0.366495	0.245072
N	-1.631658	-1.249240	0.157084
C	-0.347936	-0.818270	-0.095496
N	-0.159192	0.565764	-0.228728
C	-1.157317	1.464033	-0.137245
O	0.608905	-1.566427	-0.206674
H	-3.255165	1.719522	0.183985
H	-3.579471	-0.765376	0.442980
H	-0.885084	2.504560	-0.266257
H	2.162930	-0.574011	-0.592517
O	2.597349	0.296220	-0.568715
C	3.344019	0.359430	0.631680
H	3.790709	1.352822	0.694666
H	4.150648	-0.381461	0.641225
H	2.715009	0.198631	1.516662
H	0.812137	0.847356	-0.404942

Vibrational frequencies

27.1100	80.9885	98.4691
126.1494	154.9140	193.0385
206.1234	406.3862	521.4776
528.4359	588.0132	644.3946
774.4286	789.4284	822.8867
871.2220	937.1973	1010.6636
1014.5271	1024.6745	1051.7756
1093.7926	1136.1746	1146.8123
1186.4444	1190.5212	1267.4667
1404.3196	1465.7646	1476.9070
1490.4951	1503.7933	1521.4149
1529.3767	1621.8971	1709.6298

1804.0326	3014.4226	3078.5664
3132.1721	3152.8560	3226.9237
3261.1330	3357.9218	3652.3127



pyrimidin-2-ol + 2 CH3OH

Cartesian coordinates

C	2.846688	0.886788	0.647175
C	3.173926	-0.261039	-0.069781
N	2.271711	-1.073997	-0.592606
C	0.990179	-0.741670	-0.405634
N	0.562330	0.349335	0.251275
C	1.497478	1.145557	0.772371
O	0.110612	-1.564004	-0.920464
H	3.599101	1.537115	1.070106
H	4.212673	-0.538296	-0.230692
H	1.132354	2.020756	1.302731
H	-0.825054	-1.313158	-0.693070
O	-1.991838	1.479560	0.259728
C	-2.004931	2.394726	-0.818874
H	-1.416087	3.291313	-0.591039
H	-3.038584	2.699289	-0.987285
H	-1.618486	1.947617	-1.743007
O	-2.392105	-1.126335	-0.220496
C	-2.555874	-1.759531	1.037717
H	-1.838538	-1.382771	1.776700
H	-2.383443	-2.826511	0.894126
H	-3.570123	-1.616519	1.422885
H	-1.085435	1.115376	0.331252
H	-2.504808	-0.164330	-0.091383

Vibrational frequencies

19.9046	45.6678	53.3128
85.7609	103.2573	112.6267
120.6568	128.9419	174.0153
199.8364	206.4661	237.0045
291.7674	426.6341	530.2445
548.7521	612.8554	665.6186

778.3182	816.3409	844.6283
912.3362	980.6812	1015.6842
1025.5347	1026.4672	1040.7982
1091.9925	1104.5184	1109.4998
1129.1963	1160.3505	1165.4322
1191.7167	1195.2814	1251.5040
1296.2919	1410.1882	1425.3461
1475.7873	1486.2037	1495.8793
1500.2021	1504.1959	1505.2951
1513.7374	1530.1767	1535.6395
1554.1012	1641.0705	1686.7076
3011.3659	3019.7955	3070.1667
3090.3758	3136.9492	3143.4278
3177.0642	3183.7097	3217.5234
3246.1782	3479.4343	3572.8951

ts_2_CH_3OH

Cartesian coordinates

C	2.979906	0.717239	0.542309
C	3.115548	-0.530048	-0.082888
N	2.111341	-1.248134	-0.528452
C	0.852803	-0.750467	-0.373577
N	0.644980	0.476336	0.210811
C	1.692336	1.176329	0.657305
O	-0.126249	-1.429661	-0.778634
H	3.829204	1.279350	0.902496
H	4.104748	-0.962317	-0.224620
H	1.460797	2.133450	1.116691
H	-1.403687	-1.115384	-0.502079
O	-1.681650	1.376064	0.308933
C	-1.890118	2.279801	-0.767674
H	-1.421159	3.238966	-0.537001
H	-2.961796	2.436780	-0.899465
H	-1.469452	1.890394	-1.701386
O	-2.403970	-0.828391	-0.198901
C	-2.790852	-1.611690	0.924938
H	-2.185793	-1.369682	1.804787
H	-2.661924	-2.667583	0.684117
H	-3.841643	-1.418142	1.142812
H	-0.620256	1.023280	0.302082
H	-2.186076	0.302393	0.081388

Vibrational frequencies

-1158.7138	28.5994	63.8931
80.6494	119.9051	124.5277
138.2594	147.7228	164.2908
175.0665	200.8492	350.4366
393.8516	428.5198	547.8521
565.6094	599.1986	677.2422
693.9075	800.1629	845.6891
916.4823	1011.6544	1029.4061
1031.0894	1081.8742	1083.2212

1109.5219	1137.4761	1169.9393
1179.0740	1184.4743	1186.2272
1221.3385	1226.1690	1309.0230
1333.6355	1420.4958	1461.1199
1473.1170	1495.8990	1503.8102
1508.1185	1509.1684	1513.2854
1545.6954	1588.7766	1612.8358
1628.6161	1634.5934	1689.4239
1703.8270	1863.8035	1996.1612
3035.6137	3043.5395	3112.5632
3125.5937	3139.6934	3148.0043
3155.5747	3182.4197	3250.2942

pyrimidin-2(1H)-one + 2 CH_3OH
Cartesian coordinates

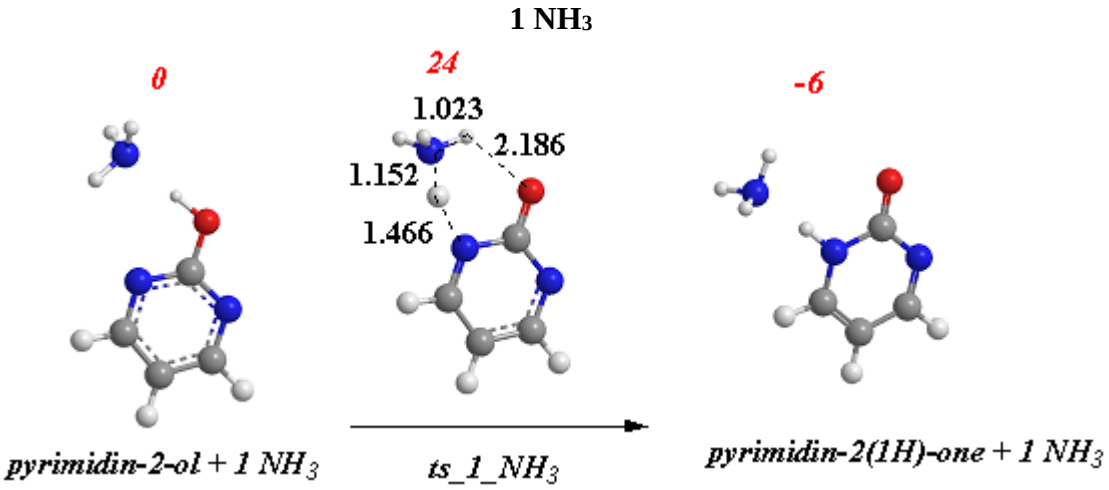
C	3.103962	0.640848	0.594233
C	3.191761	-0.597048	-0.087352
N	2.182641	-1.254412	-0.586917
C	0.917270	-0.730222	-0.454621
N	0.801093	0.498999	0.196161
C	1.853200	1.162112	0.709952
O	-0.081599	-1.292139	-0.882151
H	3.974295	1.139630	0.992952
H	4.168503	-1.060056	-0.220170
H	1.629675	2.102535	1.199465
H	-1.763076	-1.069699	-0.479749
O	-1.726450	1.612735	0.387679
C	-2.066127	2.315835	-0.794984
H	-1.541448	3.272692	-0.779214
H	-3.141797	2.512506	-0.843546
H	-1.771275	1.764845	-1.696381
O	-2.622425	-0.851584	-0.069160
C	-2.926996	-1.861209	0.872263
H	-2.154995	-1.948714	1.646534
H	-3.043362	-2.834963	0.384754
H	-3.872013	-1.599523	1.350577
H	-0.147738	0.910902	0.281165
H	-2.217537	0.763728	0.371016

Vibrational frequencies

19.3695	32.8847	58.4526
82.2926	88.8967	111.7525
125.2051	125.9222	153.0769
168.0509	204.0648	222.6372
288.0089	411.3657	520.9394
533.1788	599.2134	646.1977
778.3773	797.2122	828.7994
881.8119	952.0239	998.3166
1009.4121	1032.4200	1056.2408
1076.7641	1096.4126	1110.2382
1143.7255	1158.9508	1161.5640
1190.0070	1197.2210	1203.2995

1275.4655	1416.8214	1481.3853
1487.0425	1489.9593	1495.8268
1499.7904	1506.6619	1508.4917
1529.2227	1530.4274	1546.8374
1641.1261	1712.1207	1788.4890
3015.8477	3018.9365	3079.1245
3088.2768	3132.4918	3135.2608
3143.3896	3147.4667	3223.6326
3263.0908	3472.4576	3578.8120

4) SCRF/PCM//ωB97X-D/6-311G(d,p) for the liquid ammonia: dielectric constant is 22.63, square of the index of refraction at optical frequencies is 1.76.



pyrimidin-2-ol + 1 NH_3
Cartesian coordinates

C	2.242738	0.767116	0.000310
C	2.176876	-0.619186	0.000073
N	1.030202	-1.291243	-0.000144
C	-0.084987	-0.551610	-0.000144
N	-0.142423	0.786862	-0.000424
C	1.024420	1.426837	-0.000155
O	-1.215428	-1.226733	0.000245
H	3.184509	1.297302	0.000693
H	3.083017	-1.219029	0.000056
H	0.974627	2.512139	-0.000249
H	-2.008138	-0.598311	0.000646
N	-3.313800	0.438154	0.000028
H	-3.969294	0.350080	-0.768691
H	-3.855762	0.455723	0.857069
H	-2.857669	1.340606	-0.088204

Vibrational frequencies

56.3801	59.7820	76.8468
187.4540	240.0168	337.2112
377.8199	419.3614	545.2342
552.7853	610.4895	660.5828
816.6714	846.2419	906.9845

1013.4125	1017.1144	1028.9594
1105.2298	1108.2882	1122.8758
1148.8014	1245.8835	1294.5723
1398.1827	1456.6259	1495.8799
1543.2004	1641.4638	1655.1408
1662.9905	1670.8732	2867.1055
3173.1575	3183.2342	3249.2329
3511.0523	3630.2743	3636.7173

ts_1_NH_3

Cartesian coordinates

C	-1.980094	1.016956	-0.000008
C	-2.168425	-0.368789	-0.000006
N	-1.195295	-1.256896	-0.000001
C	0.102200	-0.791748	0.000002
N	0.349458	0.572991	0.000000
C	-0.664492	1.431770	-0.000005
O	1.064128	-1.578945	0.000006
H	-2.806440	1.713007	-0.000011
H	-3.180000	-0.773632	-0.000008
H	-0.401916	2.486849	-0.000006
H	2.931744	-0.442746	0.000010
N	2.932221	0.579904	0.000008
H	3.402085	0.929712	0.828853
H	3.402090	0.929709	-0.828835
H	1.799591	0.787529	0.000004

Vibrational frequencies

-200.0162	69.4704	148.8132
193.0028	205.2906	411.5839
464.0923	496.4567	534.3537
551.1553	601.3499	671.9579
796.2914	845.7384	874.0029
983.5905	1002.6524	1014.3237
1027.0445	1086.8794	1130.5354
1185.8839	1309.3236	1372.7440
1416.7146	1504.7198	1569.5612
1594.1867	1595.3427	1643.9745
1676.8620	1702.3430	1876.8483
3144.0378	3166.6236	3248.5192
3459.0089	3587.5177	3633.7976

pyrimidin-2(1H)-one + 1 NH_3

Cartesian coordinates

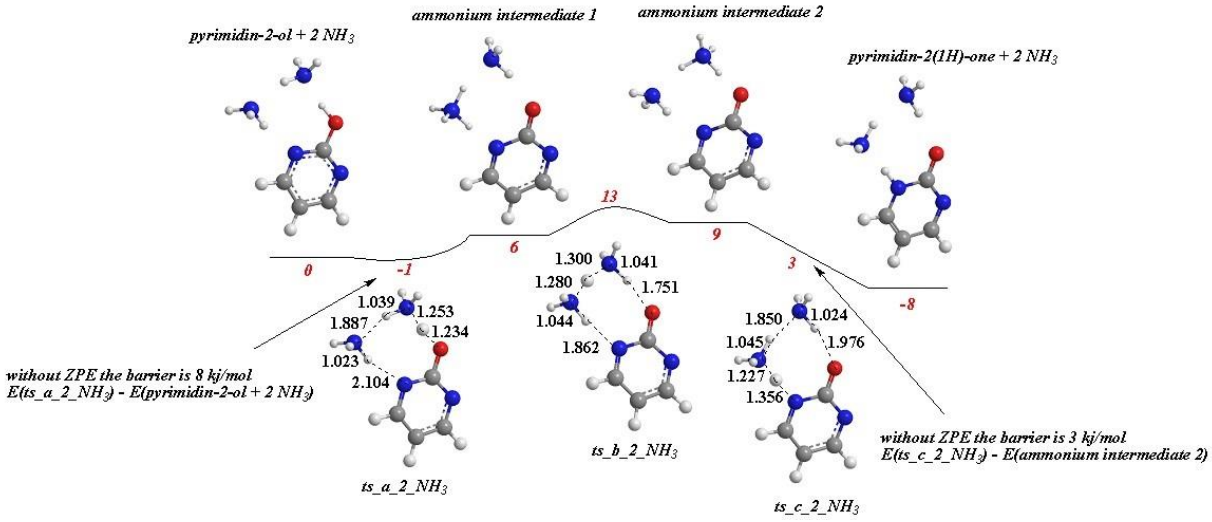
C	1.656137	-1.375330	-0.000009
C	2.227283	-0.085289	-0.000007
N	1.553965	1.037707	-0.000002
C	0.173868	0.987575	0.000002
N	-0.413933	-0.277480	0.000001
C	0.293264	-1.418375	-0.000005
O	-0.531805	1.985085	0.000008
H	2.259772	-2.269869	-0.000013

H	3.311634	0.010929	-0.000011
H	-0.281339	-2.336912	-0.000005
H	-3.652381	0.441148	0.000010
N	-3.251877	-0.491249	0.000008
H	-3.622328	-0.968880	0.814704
H	-3.622332	-0.968880	-0.814684
H	-1.458995	-0.322543	0.000004

Vibrational frequencies

54.6564	57.4921	70.3073
152.8123	206.3679	322.7233
342.4109	412.9794	516.7781
529.0784	593.3700	645.9055
795.7805	830.9331	873.5003
999.6154	1010.4032	1030.0671
1064.1020	1112.9413	1140.2106
1147.3219	1191.3921	1272.2615
1402.6557	1484.3619	1541.2048
1639.5516	1662.9571	1663.7091
1696.9778	1765.9409	2999.9068
3151.2148	3220.1197	3259.2352
3513.3187	3631.5530	3632.7818

2 NH_3



pyrimidin-2-ol + 2 NH_3

Cartesian coordinates

C	2.394217	1.124958	0.048509
C	2.719829	-0.221920	-0.042589
N	1.810286	-1.188596	-0.076667
C	0.528086	-0.801827	-0.018895
N	0.102247	0.466759	0.066068
C	1.041399	1.410693	0.099048
O	-0.355053	-1.770422	-0.050754
H	3.147892	1.898788	0.075594
H	3.757786	-0.540188	-0.091469
H	0.684620	2.434938	0.168018
N	-2.927650	-1.165370	0.096100

H	-1.323789	-1.444828	0.008553
H	-3.443844	-1.619922	-0.649792
H	-3.329950	-1.487783	0.969945
H	-3.100182	-0.155590	0.026834
N	-2.728979	1.837676	-0.115472
H	-2.811282	2.346857	-0.988299
H	-2.864716	2.509156	0.631739
H	-1.768639	1.497226	-0.051737

Vibrational frequencies

19.2254	56.2394	93.8149
140.6767	147.1245	181.2977
191.8864	212.4809	242.5171
291.0758	403.1231	404.2971
420.9885	525.3656	544.1202
609.4986	628.6244	663.9159
821.7726	845.1533	907.8326
1019.7836	1021.0778	1021.8774
1106.4172	1121.0106	1130.2315
1161.9983	1217.3080	1247.4954
1294.1049	1400.3560	1444.6644
1493.0647	1540.9100	1635.7643
1647.6910	1661.1362	1675.2693
1685.2144	1694.8356	2640.4943
3176.4043	3179.0792	3253.4809
3356.4272	3452.4190	3566.8931
3587.3168	3629.0573	3633.9205

ts_a_2_NH_3

Cartesian coordinates

C	-2.429637	1.089053	-0.000043
C	-2.706020	-0.273162	-0.000464
N	-1.770156	-1.210722	-0.000370
C	-0.478987	-0.794982	0.000193
N	-0.112699	0.512036	0.000561
C	-1.084858	1.418426	0.000441
O	0.426867	-1.703922	0.000387
H	-3.208883	1.837968	-0.000130
H	-3.735258	-0.626225	-0.000908
H	-0.766447	2.458854	0.000746
N	2.842274	-1.124450	-0.000109
H	1.610942	-1.356998	0.000239
H	3.288149	-1.524547	0.819282
H	3.287562	-1.524416	-0.819885
H	3.001868	-0.097939	-0.000115
N	2.720762	1.767732	-0.000354
H	2.909700	2.338968	0.815283
H	2.909421	2.338563	-0.816341
H	1.723753	1.538967	-0.000119

Vibrational frequencies

-894.8053	20.5563	51.2887

97.3349	133.3938	165.5002
187.9478	221.0676	265.7413
364.4590	415.9174	424.9194
466.3682	512.1151	548.7835
575.0930	648.0383	669.5137
743.1486	807.9211	849.9559
922.3586	1015.1921	1016.1454
1023.7471	1106.9291	1116.0377
1129.7492	1225.0778	1307.9740
1361.6597	1412.9116	1480.6081
1548.8843	1578.5320	1586.4667
1610.3199	1650.3310	1672.0411
1683.6174	1712.0281	1746.1049
3154.0827	3154.6870	3155.6313
3239.1668	3418.5107	3556.3095
3584.3608	3627.7735	3640.5899

ammonium intermediate 1

Cartesian coordinates

C	2.480972	1.049353	0.000127
C	2.723966	-0.320513	-0.000139
N	1.772417	-1.238993	-0.000273
C	0.473037	-0.805891	-0.000140
N	0.148789	0.526541	0.000122
C	1.142045	1.406184	0.000247
O	-0.446710	-1.672398	-0.000266
H	3.276443	1.781217	0.000231
H	3.746972	-0.694888	-0.000253
H	0.849883	2.455493	0.000458
H	-1.910033	-1.285041	-0.000144
N	-2.973522	-1.040996	-0.000072
H	-3.423516	-1.425993	-0.824900
H	-3.423452	-1.426193	0.824696
H	-3.058718	0.012551	0.000061
N	-2.663625	1.734989	0.000284
H	-2.865606	2.300306	-0.816357
H	-2.865621	2.300094	0.817068
H	-1.661205	1.516058	0.000264

Vibrational frequencies

25.3555	44.0253	88.6821
134.7820	153.7761	222.9336
235.8417	257.5903	294.0039
385.3727	426.5911	485.7992
505.1698	542.4607	569.1485
616.7324	662.0802	700.5769
800.0167	850.3960	903.6013
1003.0775	1010.4363	1011.0363
1101.0438	1113.4967	1151.0084
1202.2338	1308.8256	1399.4297
1409.1794	1481.2698	1528.0726
1552.0154	1589.0934	1604.1153

1645.7727	1658.9021	1685.6487
1749.2721	1770.4242	2299.7819
2851.1783	3138.9567	3144.8322
3245.2998	3370.9711	3552.8830
3579.2950	3625.6320	3641.8165

ts_b_2_NH_3

Cartesian coordinates

C	-2.584623	0.930811	-0.000173
C	-2.723016	-0.455685	0.000118
N	-1.709527	-1.301336	0.000264
C	-0.433855	-0.780588	0.000116
N	-0.221159	0.582925	-0.000154
C	-1.277178	1.386375	-0.000292
O	0.540035	-1.566767	0.000234
H	-3.433076	1.600629	-0.000287
H	-3.716677	-0.903307	0.000244
H	-1.063555	2.454527	-0.000511
H	2.258244	-1.227402	0.000100
N	3.225915	-0.842690	0.000032
H	3.722387	-1.169092	0.821987
H	3.722310	-1.169189	-0.821931
H	2.996593	0.437162	-0.000036
N	2.479706	1.608669	-0.000099
H	2.710047	2.155172	0.822765
H	2.710127	2.155126	-0.822971
H	1.460804	1.382055	-0.000141

Vibrational frequencies

-1057.5105	35.0159	42.2564
79.6857	148.6952	190.6465
223.0277	289.8708	319.3842
382.8694	430.3431	534.6145
537.5139	574.7381	612.1235
619.7563	638.0233	659.7105
795.3511	802.3893	847.0473
892.9512	998.8452	1008.4496
1012.5724	1093.1512	1110.5745
1184.6668	1300.7798	1313.4138
1327.6340	1414.9754	1484.6121
1560.2655	1578.4215	1606.1705
1638.3373	1660.3483	1664.7324
1686.1772	1750.9141	1794.6353
3070.9209	3131.7451	3139.3897
3144.7974	3237.3108	3560.0957
3563.3616	3636.5283	3638.0567

ammonium intermediate 2

Cartesian coordinates

C	2.640693	0.814630	0.080545
C	2.692541	-0.580155	0.044888
N	1.634054	-1.362320	-0.024622

C	0.388760	-0.767880	-0.067760
N	0.269510	0.610064	-0.030779
C	1.368703	1.352570	0.039775
O	-0.631750	-1.476165	-0.140558
H	3.529420	1.426932	0.137323
H	3.657613	-1.085514	0.076465
H	1.215409	2.430149	0.065745
H	-2.524817	-1.199126	0.066124
N	-3.462954	-0.791821	0.151176
H	-4.042024	-1.172629	-0.588545
H	-3.861962	-1.097129	1.031561
H	-2.876838	0.839065	0.012875
N	-2.235663	1.681707	-0.084074
H	-2.420547	2.165541	-0.957513
H	-2.381324	2.328131	0.685311
H	-1.219731	1.295507	-0.071482

Vibrational frequencies

21.4888	48.7570	77.5586
145.8318	165.6519	200.0243
224.7139	260.7573	289.6519
385.6933	431.8148	488.0642
518.6095	536.8791	550.0044
609.5998	663.1488	703.2808
789.0049	845.4869	889.7723
999.0216	1014.1698	1018.0449
1090.1747	1116.3673	1166.8671
1183.2249	1313.3759	1394.4234
1417.5837	1486.7711	1527.3032
1576.9163	1615.8795	1631.6992
1653.7900	1670.2942	1689.2069
1751.2584	1775.8250	2321.5229
2743.0561	3138.4108	3154.2416
3238.7788	3382.9520	3550.4827
3578.5569	3624.6530	3639.1974

ts_c_2_NH_3

Cartesian coordinates

C	2.609488	0.798165	0.107952
C	2.659362	-0.600507	0.054845
N	1.605692	-1.382541	-0.036107
C	0.357640	-0.795314	-0.085267
N	0.252602	0.584847	-0.033846
C	1.346154	1.340021	0.058553
O	-0.663747	-1.489946	-0.175028
H	3.499305	1.406019	0.182455
H	3.624629	-1.104129	0.090581
H	1.180421	2.414106	0.093976
N	-3.515561	-0.729081	0.194884
H	-2.595365	-1.163392	0.083860
H	-4.126235	-1.105747	-0.521139
H	-3.891444	-1.022547	1.089396

N	-2.067703	1.715848	-0.119949
H	-2.770760	0.953329	0.004435
H	-2.228833	2.178238	-1.009033
H	-2.179608	2.403081	0.618483
H	-0.963198	1.182916	-0.084165

Vibrational frequencies

-895.2002	23.6345	68.8227
89.7751	137.7993	156.2352
205.0586	239.5326	277.9945
387.2844	421.8023	423.6664
464.9781	523.9658	543.7321
559.3683	618.6467	683.4914
727.5402	791.3544	841.3572
901.1987	1002.5489	1018.5245
1033.8298	1089.0447	1131.3394
1143.9434	1188.6938	1314.7780
1370.0006	1414.6165	1493.7378
1565.7758	1586.3312	1609.0193
1650.2332	1670.1109	1681.9318
1689.3120	1720.0510	1797.3060
3059.4867	3146.2087	3174.4123
3248.9617	3406.0275	3553.3715
3580.6041	3627.7404	3637.4290

pyrimidin-2(1H)-one + 2 NH_3

Cartesian coordinates

C	2.624720	0.833441	0.060128
C	2.694560	-0.573890	0.032090
N	1.660649	-1.377330	-0.018964
C	0.395358	-0.831782	-0.049184
N	0.296912	0.555326	-0.020795
C	1.368034	1.362722	0.031226
O	-0.617387	-1.521761	-0.099020
H	3.508508	1.451483	0.101779
H	3.670070	-1.055915	0.054342
H	1.160676	2.426222	0.048406
N	-3.594975	-0.826332	0.105801
H	-2.636064	-1.169994	0.043820
H	-4.112598	-1.242869	-0.660106
H	-3.992005	-1.198108	0.961462
N	-2.198325	1.839053	-0.061649
H	-2.870670	1.064164	0.005061
H	-2.403105	2.354380	-0.910885
H	-2.370524	2.469108	0.714243
H	-0.661051	0.997657	-0.042275

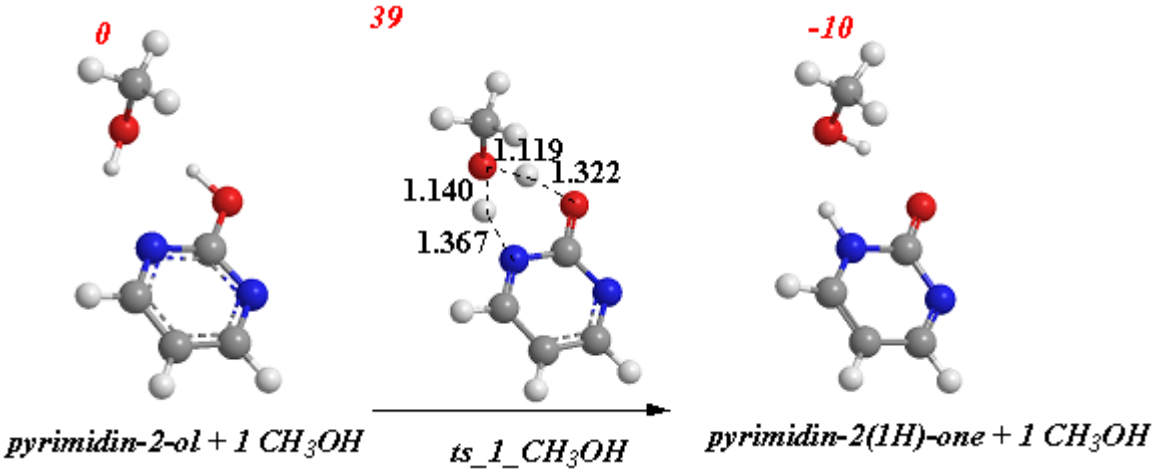
Vibrational frequencies

7.6109	63.9381	77.1317
137.2239	147.1652	154.6715
200.6854	208.1662	214.8704
280.5675	370.1099	381.9168

414.3185	518.0901	527.4138
577.3792	602.2404	646.2437
797.8220	828.5198	879.9862
995.6782	1007.1296	1021.1121
1066.5796	1125.3504	1137.3580
1151.8133	1186.9065	1198.5220
1277.1579	1408.5515	1485.2109
1546.0307	1634.7147	1654.4919
1665.3976	1687.7102	1696.9027
1699.5577	1747.8478	2826.8746
3163.1396	3222.9036	3258.2536
3338.3550	3460.3634	3566.1693
3588.7060	3630.3220	3632.2214

5) SCRF/PCM//ωB97X-D/6-311G(d,p) for the liquid methanol: dielectric constant is 32.613, square of the index of refraction at optical frequencies is 1.765709.

1 CH_3OH



pyrimidin-2-ol + 1 CH_3OH
Cartesian coordinates

C	-2.429411	1.013882	0.102411
C	-2.594140	-0.354906	0.264964
N	-1.590801	-1.222946	0.169040
C	-0.394637	-0.701761	-0.096585
N	-0.118272	0.595256	-0.274888
C	-1.142587	1.441610	-0.172372
O	0.601927	-1.570579	-0.190922
H	-3.256071	1.704811	0.183836
H	-3.571207	-0.777109	0.480016
H	-0.914157	2.492274	-0.317887
H	1.435487	-1.079760	-0.379766
O	2.625206	0.179397	-0.578370
C	3.270542	0.430581	0.665404
H	3.729122	1.423620	0.678972
H	4.052622	-0.318702	0.786520
H	2.570406	0.349169	1.504037
H	1.841637	0.752550	-0.623386

Vibrational frequencies

38.8527	73.0826	100.6892
131.3282	182.4524	203.7108
212.1805	422.6913	507.5472
546.4304	608.6317	660.4186
715.3087	825.7026	842.6377
881.8907	904.4527	1024.4509
1031.4491	1037.0152	1067.6125
1112.1834	1125.1500	1133.3345
1183.5763	1251.3193	1291.7820
1394.7921	1431.7885	1452.1028
1481.7451	1491.9772	1495.2241
1509.9083	1532.0069	1652.9968
1674.0638	3029.9191	3099.1800
3144.1396	3189.9822	3202.2193
3252.9622	3377.6336	3661.8811

ts_1_CH_3OH

Cartesian coordinates

C	-2.351250	1.010537	0.086873
C	-2.515322	-0.367676	0.234995
N	-1.530051	-1.247703	0.159417
C	-0.291796	-0.763005	-0.077721
N	-0.054357	0.577046	-0.236539
C	-1.065383	1.440832	-0.154094
O	0.704610	-1.553672	-0.163719
H	-3.181511	1.697751	0.155237
H	-3.503654	-0.779072	0.424498
H	-0.818744	2.488246	-0.287825
H	1.751312	-0.778387	-0.392346
O	2.309137	0.180305	-0.543558
C	3.126914	0.469078	0.595326
H	3.565563	1.458067	0.468468
H	3.920951	-0.274559	0.654053
H	2.536486	0.444725	1.515924
H	1.291503	0.686164	-0.452219

Vibrational frequencies

-1328.8280	71.3130	127.7169
153.5124	166.5848	209.7726
376.4301	409.1653	422.2629
544.8915	600.3704	646.3344
692.8644	813.4849	844.6264
905.4517	989.5637	1025.9181
1039.2361	1053.8593	1080.8396
1103.3995	1143.6831	1168.5139
1205.5058	1231.7909	1319.6150
1357.3177	1417.1271	1490.7758
1495.9198	1503.5341	1508.8104
1542.5228	1564.5340	1612.1965
1682.5718	1738.2249	2106.6876
3052.6885	3137.9985	3165.2549

3172.3027	3213.3304	3256.6438

pyrimidin-2(1H)-one + 1 CH_3OH

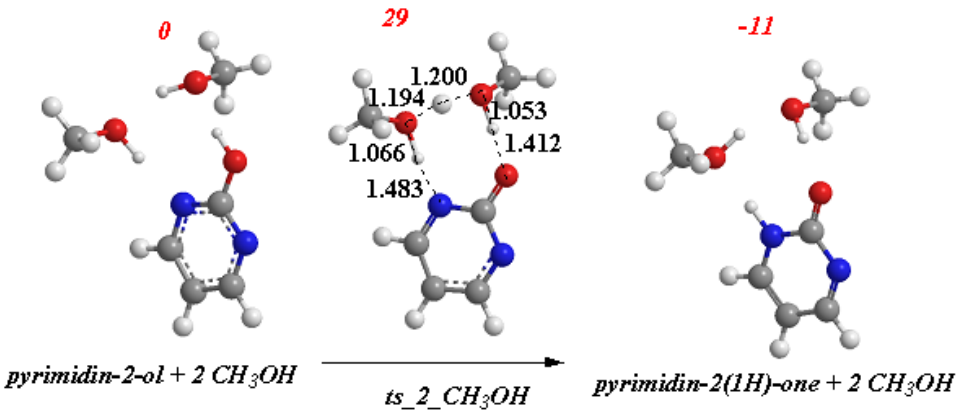
Cartesian coordinates

C	-2.403774	1.042108	0.103851
C	-2.574445	-0.347970	0.270847
N	-1.619478	-1.241240	0.178356
C	-0.346113	-0.818083	-0.101973
N	-0.151244	0.549749	-0.276295
C	-1.138542	1.459257	-0.177149
O	0.609111	-1.586245	-0.204263
H	-3.226280	1.734915	0.191782
H	-3.565864	-0.736090	0.493352
H	-0.860037	2.493369	-0.331435
H	2.163740	-0.618772	-0.546237
O	2.644884	0.225827	-0.586754
C	3.256445	0.422894	0.679316
H	3.754541	1.392761	0.660283
H	4.005018	-0.348417	0.888438
H	2.518982	0.425277	1.491089
H	0.811558	0.831502	-0.482908

Vibrational frequencies

50.5463	78.5733	107.8970
134.9092	170.9643	188.6398
204.1966	409.7706	521.9950
527.7585	591.8620	649.1446
772.9974	800.2110	826.2546
881.5157	919.9944	1013.8598
1030.4243	1035.6710	1066.8685
1075.4892	1130.9855	1142.3274
1190.7262	1206.6531	1262.1507
1393.2852	1451.9744	1473.3611
1487.4288	1497.9837	1513.8396
1514.1241	1617.3357	1695.2129
1742.4981	3018.9256	3080.3311
3139.7076	3172.0311	3244.9488
3269.2468	3402.4542	3630.4164

2 CH_3OH



pyrimidin-2-ol + 2 CH_3OH

Cartesian coordinates

C	2.861913	0.869309	0.634362
C	3.178224	-0.279337	-0.080190
N	2.260210	-1.090726	-0.592547
C	0.986510	-0.746787	-0.389832
N	0.569546	0.340811	0.270784
C	1.514714	1.136250	0.777927
O	0.092497	-1.568357	-0.900956
H	3.621667	1.518033	1.045408
H	4.213486	-0.560547	-0.249435
H	1.163617	2.014732	1.310007
H	-0.839711	-1.305593	-0.669032
O	-1.983141	1.485507	0.258892
C	-1.963993	2.398666	-0.828509
H	-1.336212	3.267622	-0.604477
H	-2.985126	2.742872	-0.994888
H	-1.598547	1.928068	-1.748248
O	-2.413381	-1.111417	-0.237830
C	-2.596277	-1.724566	1.033622
H	-1.870783	-1.353250	1.765755
H	-2.449486	-2.797184	0.906797
H	-3.607116	-1.549356	1.412077
H	-1.078519	1.120624	0.350164
H	-2.495912	-0.143682	-0.116913

Vibrational frequencies

9.2821	27.9104	49.8336
55.2557	93.2123	111.1870
122.6104	126.4663	172.5716
202.3061	205.8599	230.6566
288.7829	424.3800	527.7804
546.3766	612.2020	664.6405
758.8523	823.2687	842.7446
908.6930	970.1264	1014.2729
1026.4024	1027.4369	1036.2829
1070.5529	1088.6119	1113.4098
1128.5213	1150.8388	1157.9636
1190.3105	1191.9738	1249.2765
1288.7010	1400.9546	1416.0411
1470.2331	1478.4310	1487.1862
1488.5656	1494.8417	1497.0579
1502.7225	1517.2523	1523.2418
1533.2131	1643.7365	1672.9714
3021.0704	3026.4512	3083.6159
3099.0467	3140.8951	3145.1275
3178.0430	3189.5398	3197.8664
3253.8002	3459.8367	3534.3917

ts_2_CH_3OH

Cartesian coordinates

C	3.008151	0.747306	0.497912

C	3.157500	-0.518730	-0.069717
N	2.151071	-1.269018	-0.477707
C	0.889507	-0.773859	-0.334258
N	0.667344	0.467053	0.203631
C	1.710524	1.194761	0.606719
O	-0.085102	-1.483932	-0.713526
H	3.851694	1.337534	0.824749
H	4.150615	-0.944263	-0.198565
H	1.477003	2.168234	1.028026
H	-1.433823	-1.140797	-0.477230
O	-1.712318	1.361103	0.304855
C	-1.918897	2.328323	-0.729430
H	-1.431130	3.261509	-0.446970
H	-2.989846	2.497705	-0.832276
H	-1.511563	1.974938	-1.680430
O	-2.416028	-0.842736	-0.241014
C	-2.882513	-1.605374	0.876211
H	-2.273110	-1.413594	1.763243
H	-2.836698	-2.665553	0.626929
H	-3.916223	-1.325843	1.074531
H	-0.692559	1.050635	0.305663
H	-2.201316	0.303206	0.043719

Vibrational frequencies

-866.6439	25.6281	56.9058
59.3135	80.6873	114.6102
130.7189	143.3873	153.3905
174.4318	195.2982	294.3708
381.1816	427.9852	546.7644
562.1052	593.8646	654.8578
678.1861	807.7853	847.3021
910.4690	1019.0353	1023.2534
1037.4693	1070.6259	1083.9988
1097.2574	1120.9925	1153.4387
1161.1228	1162.8841	1176.0394
1213.4582	1217.6903	1282.6242
1328.0678	1420.5698	1448.7678
1472.2413	1487.0519	1491.5331
1493.6779	1495.6591	1501.4347
1527.7415	1566.5211	1589.3459
1600.2699	1642.1586	1669.3178
1811.1090	2049.9430	2231.9400
3056.2859	3058.4220	3140.3885
3140.4389	3155.6913	3166.7693
3168.1324	3189.7875	3248.5913

pyrimidin-2(1H)-one + 2 CH_3OH

Cartesian coordinates

C	3.023918	0.683701	0.664708
C	3.171977	-0.493807	-0.094616
N	2.188905	-1.148306	-0.664958
C	0.911646	-0.673323	-0.524242

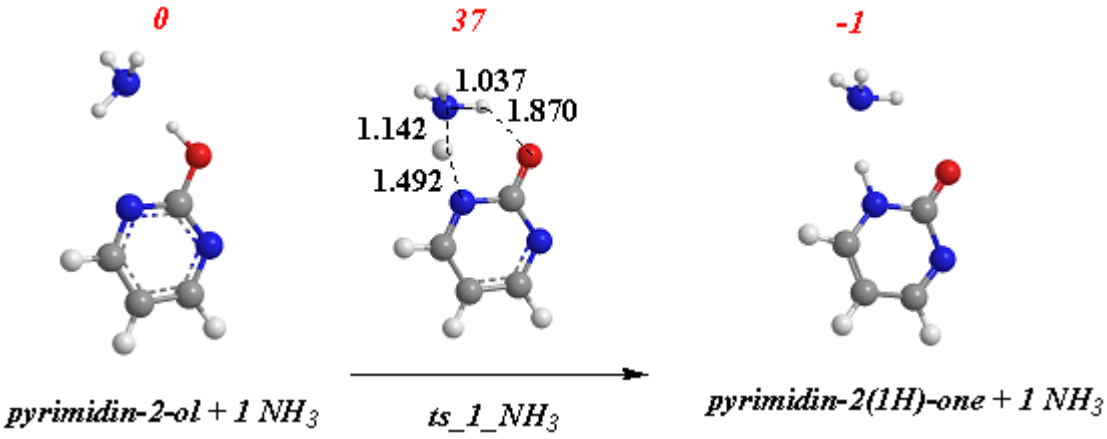
N	0.735261	0.491735	0.207588
C	1.751723	1.154494	0.789689
O	-0.060219	-1.242480	-1.025673
H	3.866710	1.183905	1.116181
H	4.165432	-0.913800	-0.234926
H	1.487413	2.050574	1.336449
H	-1.722635	-1.138549	-0.542701
O	-1.854624	1.513703	0.366072
C	-2.116210	2.291889	-0.793872
H	-1.616169	3.253004	-0.670025
H	-3.188778	2.470428	-0.916964
H	-1.732199	1.810120	-1.700457
O	-2.597578	-1.029227	-0.119737
C	-2.610691	-1.855788	1.034751
H	-1.833704	-1.564689	1.751370
H	-2.467583	-2.908583	0.771128
H	-3.584207	-1.746363	1.513750
H	-0.227255	0.867073	0.294533
H	-2.310992	0.653917	0.259449

Vibrational frequencies

26.2845	47.3611	60.9577
88.0337	96.5240	121.6379
126.8465	160.4419	165.2987
180.3182	202.8063	221.8914
280.8838	412.1056	521.5619
530.1282	600.7257	649.4143
747.5935	809.7970	830.3966
889.1691	950.8206	996.7116
1011.1168	1041.5469	1065.3535
1071.8091	1076.0261	1088.8815
1142.3002	1151.7590	1158.0474
1193.8807	1197.3685	1216.1463
1267.8417	1404.3431	1470.8477
1483.0799	1485.3834	1490.6799
1495.9382	1501.9168	1504.2248
1518.8622	1523.0024	1534.1995
1630.4160	1698.6601	1730.5521
3021.7773	3023.5737	3087.1751
3090.9554	3134.7091	3137.6787
3162.1598	3166.2598	3234.5142
3266.1991	3481.3197	3547.8518

6) SCRF/PCM//ωB97X-D/6-311G(d,p) for the solid ammonia: dielectric constant is 3.4, square of the index of refraction at optical frequencies is 1.96.

1 NH_3



pyrimidin-2-ol + 1 NH_3
Cartesian coordinates

C	-2.208073	0.800280	0.000000
C	-2.174633	-0.588239	0.000000
N	-1.046634	-1.287698	0.000000
C	0.086120	-0.576193	0.000000
N	0.175827	0.761905	0.000000
C	-0.974730	1.429896	0.000000
O	1.199726	-1.277244	0.000000
H	-3.137089	1.352818	0.000000
H	-3.094844	-1.166712	0.000000
H	-0.897413	2.513803	0.000000
H	1.997322	-0.665708	0.000000
N	3.264821	0.456883	0.000000
H	3.861310	0.491674	0.818553
H	3.861308	0.491675	-0.818555
H	2.681399	1.288310	0.000001

Vibrational frequencies

56.5202	106.9027	114.3079
184.7655	241.6251	316.3031
405.5765	420.7966	545.4957
557.8673	609.6505	662.3836
816.8395	846.9653	907.0107
1009.1818	1017.8102	1024.4165
1084.7768	1109.0217	1121.1822
1126.3315	1246.5743	1297.1279
1403.0471	1451.8330	1505.7883
1537.3136	1641.3477	1658.8092
1672.9282	1674.1914	3003.4411
3173.3599	3179.0907	3244.0624
3509.1776	3630.7504	3645.9413

ts_1_NH_3
Cartesian coordinates

C	-2.029894	0.941904	-0.000009
C	-2.139072	-0.453822	-0.000006
N	-1.118670	-1.283626	0.000000
C	0.146436	-0.745627	0.000003
N	0.321648	0.631667	-0.000001
C	-0.741787	1.430527	-0.000007
O	1.151358	-1.483232	0.000009
H	-2.894975	1.589414	-0.000014
H	-3.125584	-0.916264	-0.000008
H	-0.540789	2.499318	-0.000009
H	2.704681	-0.442177	0.000010
N	2.889781	0.578464	0.000007
H	3.395751	0.860732	0.832302
H	3.395756	0.860727	-0.832287
H	1.790891	0.890674	0.000003

Vibrational frequencies

-267.6022	71.2314	148.2485
260.8604	289.9828	408.4478
450.8708	484.8806	533.5986
558.7013	603.3344	672.7284
794.8131	845.5061	880.6551
990.0535	995.9568	1010.0798
1024.8951	1083.7414	1132.5398
1188.5255	1309.7021	1378.4239
1426.9311	1505.6868	1573.4527
1593.0458	1621.4770	1635.1519
1686.9587	1700.2540	1987.9309
3145.7532	3168.2777	3238.5119
3246.7624	3568.2082	3644.6003

pyrimidin-2(1H)-one + 1 NH_3

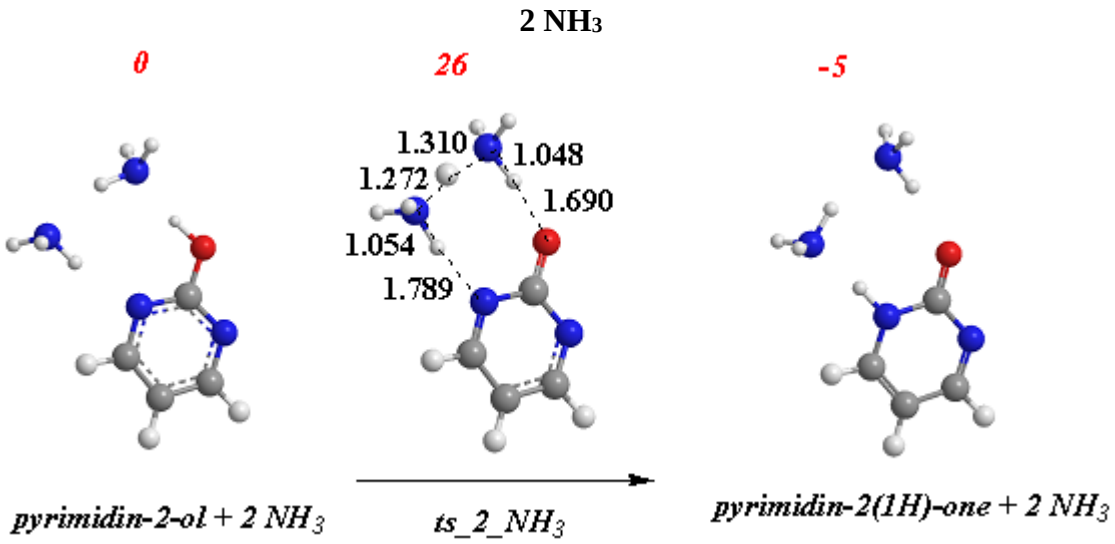
Cartesian coordinates

C	-1.949035	1.097050	-0.000010
C	-2.201523	-0.294125	-0.000006
N	-1.287668	-1.228066	0.000000
C	0.042864	-0.857771	0.000003
N	0.317689	0.514061	0.000000
C	-0.635977	1.459586	-0.000007
O	0.964271	-1.657519	0.000009
H	-2.745896	1.824960	-0.000014
H	-3.233452	-0.642019	-0.000009
H	-0.294162	2.487763	-0.000009
H	3.044055	-0.421172	0.000010
N	3.149983	0.590780	0.000007
H	3.694730	0.841655	0.816983
H	3.694735	0.841651	-0.816966
H	1.327823	0.761454	0.000002

Vibrational frequencies

63.8792	95.9117	136.0125
148.1382	207.3339	312.5047

406.6641	419.9522	518.9348
521.0554	590.2210	647.2885
794.5339	827.7122	870.2391
987.1825	1012.0367	1016.8599
1057.5593	1080.3654	1127.5163
1143.1632	1187.8466	1268.6182
1400.7698	1482.0080	1535.4881
1629.1760	1664.1669	1679.0881
1700.6853	1789.5758	3110.6577
3152.6989	3220.9731	3266.4865
3496.0274	3615.4617	3642.5745



pyrimidin-2-ol + 2 NH3
Cartesian coordinates

C	-2.401818	1.117519	-0.039207
C	-2.719733	-0.233429	0.032784
N	-1.807154	-1.194491	0.060396
C	-0.526195	-0.801635	0.015417
N	-0.106577	0.471336	-0.050813
C	-1.050642	1.409845	-0.077607
O	0.360391	-1.764917	0.040334
H	-3.159526	1.887768	-0.061386
H	-3.756119	-0.559281	0.070898
H	-0.698168	2.436934	-0.131504
H	1.321442	-1.434182	-0.006237
N	2.950372	-1.153301	-0.076771
H	3.452079	-1.596860	0.685022
H	3.361837	-1.492784	-0.939445
H	3.122097	-0.142471	-0.022429
N	2.714557	1.837728	0.091236
H	2.799762	2.356507	0.957635
H	2.847483	2.496456	-0.667177
H	1.757924	1.484550	0.035290

Vibrational frequencies

18.0604	57.2664	94.7481

140.4010	152.8767	179.4222
199.6170	214.9520	241.5487
295.6878	404.0248	412.6375
421.9901	527.0846	544.4746
610.3818	633.1787	664.8978
819.4663	845.7591	909.2094
1014.7245	1017.3489	1019.3321
1104.5181	1120.3168	1130.6929
1151.7506	1216.7020	1248.8060
1295.8839	1403.4310	1445.3040
1500.4368	1545.1862	1636.5441
1651.1581	1666.8283	1679.4291
1693.6146	1705.1928	2767.6880
3171.9827	3172.7651	3251.0529
3358.8678	3444.4087	3569.9061
3588.5961	3632.9663	3639.4001

ts_2_NH_3

Cartesian coordinates

C	-2.595580	0.894391	-0.000071
C	-2.698272	-0.497843	0.000110
N	-1.667550	-1.317115	0.000169
C	-0.405242	-0.766974	0.000044
N	-0.226556	0.602899	-0.000125
C	-1.302388	1.381554	-0.000179
O	0.587333	-1.526641	0.000086
H	-3.461273	1.541838	-0.000117
H	-3.680786	-0.969857	0.000214
H	-1.114164	2.454858	-0.000319
H	2.245451	-1.201667	0.000131
N	3.223039	-0.823548	0.000145
H	3.714176	-1.157146	0.822234
H	3.714266	-1.157320	-0.821821
H	2.970171	0.461585	-0.000007
N	2.421545	1.609365	-0.000162
H	2.634528	2.162329	0.823049
H	2.634604	2.162144	-0.823477
H	1.399907	1.348394	-0.000178

Vibrational frequencies

-998.5505	27.0064	42.0377
90.6936	144.3725	223.7387
240.5733	293.8577	324.6810
396.7848	433.4763	537.1260
540.9514	581.7385	614.6282
638.4405	640.4566	661.9200
791.5865	818.1313	847.1424
895.5622	992.3124	1005.2428
1015.3022	1089.2923	1114.7906
1187.2759	1315.8114	1326.1818
1365.1503	1419.6651	1487.9323
1556.4329	1581.0063	1615.9876

1644.1487	1672.9877	1678.5752
1696.9228	1756.0462	1802.3773
2898.3985	3013.8637	3137.9828
3140.2966	3231.8828	3556.9436
3561.3114	3637.0260	3639.3461

pyrimidin-2(1H)-one + 2 NH_3
Cartesian coordinates

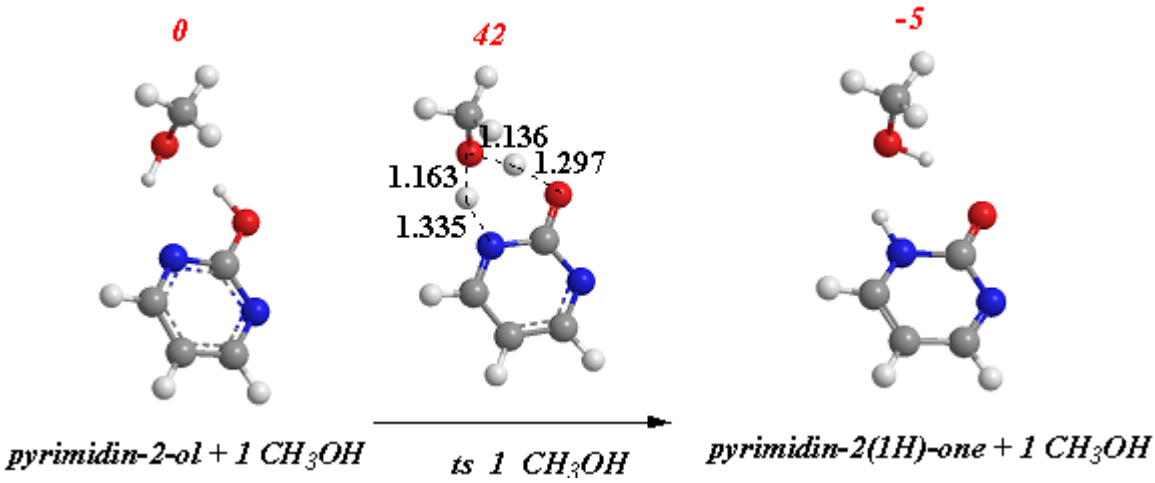
C	2.616177	0.850754	0.000252
C	2.696268	-0.559251	0.000088
N	1.671827	-1.371046	-0.000120
C	0.398112	-0.839283	-0.000186
N	0.290055	0.551165	-0.000045
C	1.355650	1.368102	0.000166
O	-0.607347	-1.534698	-0.000358
H	3.495766	1.476417	0.000420
H	3.676453	-1.033296	0.000130
H	1.138868	2.430196	0.000266
H	-2.608818	-1.193590	0.000174
N	-3.565820	-0.837622	0.000426
H	-4.029897	-1.225756	-0.813007
H	-4.029375	-1.225506	0.814277
H	-2.870646	1.041564	-0.000035
N	-2.221961	1.841276	-0.000291
H	-2.431120	2.406949	-0.815575
H	-2.431104	2.407468	0.814637
H	-0.667306	0.984797	-0.000133

Vibrational frequencies

9.4187	62.3151	78.0036
132.8328	147.4155	150.6618
208.5669	212.5494	234.5803
295.3661	386.6852	397.6762
414.8201	519.2528	527.0468
586.0371	606.5596	645.9426
795.5058	827.7814	876.7769
990.6484	1007.6747	1014.3725
1059.8374	1137.1287	1141.1814
1142.0623	1192.8536	1205.9439
1278.2836	1411.7088	1485.3240
1545.5088	1637.3792	1656.9072
1672.0256	1699.1733	1705.0006
1713.2045	1769.8711	2918.6644
3158.1110	3216.4327	3253.0354
3323.8876	3451.3657	3565.6087
3585.7702	3632.4379	3633.2907

7) SCRF/PCM//ωB97X-D/6-311G(d,p) for the solid methanol: dielectric constant is 3.0, square of the index of refraction at optical frequencies is 1.5876.

1 CH_3OH



pyrimidin-2-ol + 1 CH_3OH
Cartesian coordinates

C	-2.407359	1.040666	0.105943
C	-2.575041	-0.354322	0.265348
N	-1.622329	-1.244336	0.172298
C	-0.344715	-0.820057	-0.102611
N	-0.151694	0.554630	-0.263237
C	-1.142234	1.460794	-0.164885
O	0.609830	-1.580289	-0.210968
H	-3.232542	1.730762	0.192688
H	-3.567132	-0.745463	0.482424
H	-0.866023	2.497128	-0.311785
H	2.171075	-0.599954	-0.577063
O	2.626816	0.259379	-0.582298
C	3.275596	0.396106	0.671138
H	3.755431	1.375353	0.692292
H	4.045567	-0.369951	0.810082
H	2.566674	0.333996	1.506302
H	0.814472	0.834224	-0.461847

Vibrational frequencies

45.2840	79.8135	103.5343
140.0990	165.4121	191.0545
203.2479	408.9354	521.8115
527.3425	589.8115	646.8232
766.5649	795.6168	825.0865
876.6106	930.4811	1012.2798
1024.6403	1030.1591	1059.7897
1082.2444	1133.4193	1143.5049
1187.4932	1199.5047	1260.7834
1398.6860	1459.4729	1473.9464
1487.0323	1501.2097	1515.8520
1520.0298	1618.7396	1701.4894
1770.1563	3016.0026	3078.5556
3137.7181	3164.4351	3236.1116
3265.8482	3378.1366	3645.7369

ts_1_CH_3OH

Cartesian coordinates

C	-2.349839	1.006922	0.086054
C	-2.507936	-0.374857	0.233778
N	-1.523368	-1.250643	0.158971
C	-0.285403	-0.764076	-0.077766
N	-0.053035	0.579837	-0.231608
C	-1.066902	1.441580	-0.151517
O	0.712965	-1.546312	-0.167877
H	-3.183491	1.690374	0.152691
H	-3.495167	-0.790147	0.422537
H	-0.822225	2.489800	-0.284668
H	1.733883	-0.780610	-0.400061
O	2.304037	0.191016	-0.546391
C	3.113209	0.463096	0.595844
H	3.567353	1.447946	0.482477
H	3.901001	-0.287843	0.661617
H	2.519067	0.440217	1.515814
H	1.259620	0.692280	-0.446163

Vibrational frequencies

-1454.2062	73.4664	126.9868
159.2242	170.8097	207.6913
383.5779	422.4357	432.7604
544.5054	602.2411	653.5221
703.6648	810.7568	843.9223
903.5685	979.4832	1020.2164
1035.8366	1053.6818	1088.0133
1115.2169	1147.0109	1173.3541
1204.6994	1233.8951	1321.2741
1378.4992	1420.8475	1494.2491
1500.8527	1509.6657	1517.7209
1551.2893	1570.3561	1614.8834
1686.0582	1742.6226	2066.0282
3040.3411	3123.0218	3151.5788
3168.5585	3208.9758	3254.6614

pyrimidin-2(1H)-one + 1 CH_3OH

Cartesian coordinates

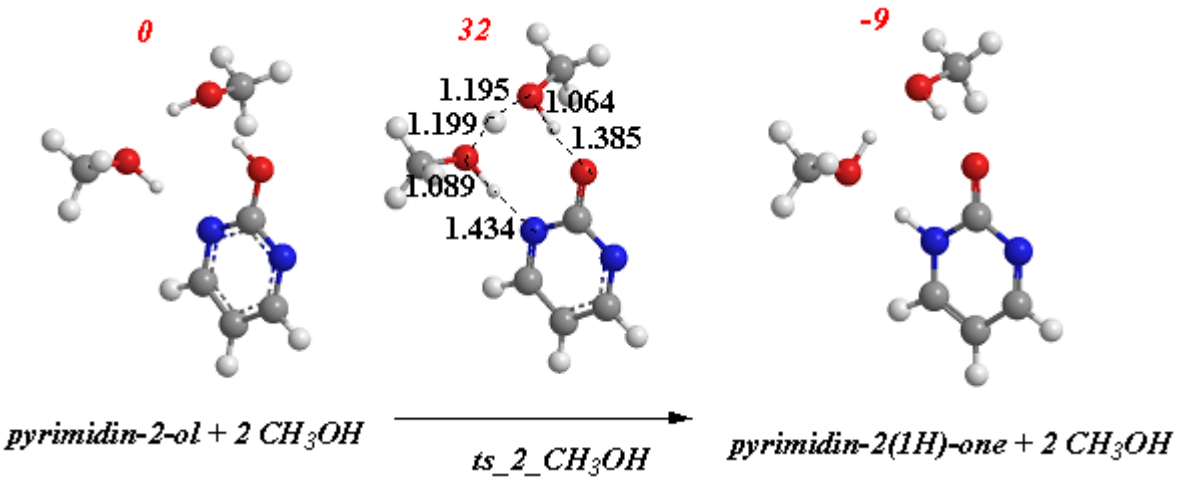
C	-2.426918	1.012915	0.102577
C	-2.588072	-0.357151	0.268284
N	-1.586463	-1.223198	0.171207
C	-0.390115	-0.703169	-0.099261
N	-0.115955	0.596281	-0.277409
C	-1.141312	1.440621	-0.174475
O	0.604095	-1.569600	-0.197227
H	-3.254658	1.702869	0.183946
H	-3.563820	-0.781448	0.487239
H	-0.913644	2.491645	-0.321739
H	1.435877	-1.082002	-0.396989
O	2.627646	0.188568	-0.579978
C	3.252258	0.426749	0.674043

H	3.706338	1.421975	0.709272
H	4.037423	-0.319210	0.796580
H	2.541765	0.329487	1.503062
H	1.838677	0.753562	-0.627330

Vibrational frequencies

49.8048	76.3939	108.0110
135.4018	184.1126	204.8959
215.8039	424.1675	512.8821
547.4916	608.9854	661.4610
732.1296	823.4301	843.7272
893.0450	906.0336	1023.7647
1027.0748	1033.0210	1076.3354
1110.9920	1125.1790	1136.9112
1186.7174	1251.9292	1294.7114
1401.1131	1434.9467	1456.2259
1486.4561	1498.9393	1503.9737
1514.9309	1535.2221	1652.9367
1678.9247	3024.9451	3092.1738
3142.8914	3185.6287	3195.9923
3249.9341	3404.5804	3669.2283

2 CH_3OH



pyrimidin-2-ol + 2 CH_3OH

Cartesian coordinates

C	2.854511	0.859252	0.654194
C	3.169976	-0.276447	-0.083896
N	2.254948	-1.076469	-0.612718
C	0.979546	-0.737979	-0.405825
N	0.563250	0.340099	0.274338
C	1.507706	1.123955	0.799129
O	0.086988	-1.547727	-0.929285
H	3.614451	1.498459	1.080074
H	4.205419	-0.555498	-0.258225
H	1.154385	1.991955	1.347776
H	-0.844269	-1.292087	-0.687571
O	-1.976521	1.502332	0.270057
C	-1.963551	2.375997	-0.846744

H	-1.252422	3.196851	-0.701967
H	-2.962322	2.800542	-0.952679
H	-1.707291	1.850872	-1.774678
O	-2.410177	-1.101553	-0.217349
C	-2.569094	-1.740301	1.042268
H	-1.840108	-1.373522	1.773906
H	-2.409189	-2.808151	0.892511
H	-3.577689	-1.587089	1.436743
H	-1.078394	1.119317	0.350854
H	-2.506843	-0.138326	-0.080230

Vibrational frequencies

18.8388	45.7051	54.0037
86.3059	105.4813	113.4177
124.8919	129.4705	177.8682
203.6277	208.0112	234.8620
288.5788	425.0692	528.4769
547.0723	612.5629	664.9163
767.6864	818.2062	843.8854
910.7220	984.5267	1019.5250
1026.5804	1029.3039	1035.2142
1079.8688	1094.4719	1111.7214
1128.4787	1155.3692	1162.0290
1192.6031	1195.1708	1250.8167
1291.8997	1405.6957	1421.6204
1472.8253	1485.6612	1495.3653
1496.8543	1499.8551	1501.2190
1508.9533	1524.0347	1529.9029
1541.5310	1642.8295	1678.8338
3017.7367	3023.7099	3079.1816
3095.4401	3135.4652	3145.4336
3183.0457	3190.1091	3198.1215
3251.4513	3466.1917	3554.5732

ts_2_CH_3OH

Cartesian coordinates

C	2.988638	0.726563	0.538123
C	3.132482	-0.520983	-0.077299
N	2.128148	-1.247229	-0.520962
C	0.867895	-0.751380	-0.370053
N	0.651706	0.474046	0.209744
C	1.695983	1.179779	0.650910
O	-0.108078	-1.437906	-0.778236
H	3.834286	1.296108	0.895039
H	4.123776	-0.948986	-0.214133
H	1.463195	2.138719	1.105364
H	-1.427957	-1.125458	-0.497239
O	-1.701555	1.366259	0.304717
C	-1.908761	2.292726	-0.760753
H	-1.428895	3.240752	-0.512920
H	-2.979936	2.455955	-0.878632
H	-1.495515	1.910916	-1.699199

O	-2.412414	-0.842065	-0.209067
C	-2.805385	-1.615620	0.925390
H	-2.176019	-1.390862	1.791376
H	-2.716662	-2.674445	0.681629
H	-3.844457	-1.384736	1.158362
H	-0.663196	1.037715	0.303671
H	-2.196333	0.299796	0.067987

Vibrational frequencies

-974.4976	24.6853	62.4095
81.4558	88.0777	118.3514
138.2924	148.5158	160.5807
175.4333	198.5538	320.7731
392.0289	428.8095	547.7559
564.5531	597.1269	667.5825
684.5738	803.3763	847.0244
912.9972	1018.1155	1026.8087
1035.1437	1076.2527	1088.0922
1098.8344	1128.8617	1165.0130
1170.5069	1174.4195	1177.6071
1216.7866	1223.3292	1293.5287
1342.5197	1422.2356	1450.0115
1475.3477	1492.8235	1495.8593
1499.4870	1501.4662	1507.5705
1537.3301	1581.8863	1601.4517
1609.0161	1664.5358	1674.1686
1750.2659	1899.7027	2147.5066
3048.0846	3052.1090	3129.3748
3135.0245	3152.6299	3156.2997
3161.8719	3185.6225	3251.5044

pyrimidin-2(1H)-one + 2 CH_3OH

Cartesian coordinates

C	3.080893	0.649624	0.613655
C	3.184998	-0.570877	-0.089186
N	2.180047	-1.227359	-0.608472
C	0.913594	-0.714840	-0.472517
N	0.780844	0.494043	0.202847
C	1.824062	1.157722	0.734739
O	-0.078801	-1.279910	-0.924362
H	3.944140	1.149224	1.025965
H	4.165746	-1.022659	-0.224556
H	1.590810	2.086185	1.241040
H	-1.755509	-1.080350	-0.501302
O	-1.767362	1.589025	0.386559
C	-2.060970	2.317021	-0.796420
H	-1.551746	3.279615	-0.731929
H	-3.135731	2.498698	-0.892878
H	-1.712230	1.792285	-1.693752
O	-2.625475	-0.897900	-0.095019
C	-2.835635	-1.862499	0.921364
H	-2.053224	-1.826664	1.688521

H	-2.870359	-2.873932	0.503635
H	-3.795787	-1.649260	1.392852
H	-0.171170	0.896286	0.290743
H	-2.249727	0.737146	0.333800

Vibrational frequencies

26.0978	44.3856	59.1002
83.9451	92.4519	113.4563
122.8351	129.9077	136.3054
174.6783	203.1421	222.9900
284.7058	411.6228	521.5659
532.8524	600.0108	648.1213
763.3668	803.6996	830.1876
885.6290	949.0090	1000.4024
1010.3744	1039.2794	1063.4418
1072.3769	1086.1819	1099.4402
1143.1150	1155.5889	1159.3530
1192.6693	1194.4926	1210.1433
1272.4041	1412.0408	1475.1346
1484.1475	1486.9952	1493.1686
1496.5859	1502.5553	1505.0798
1522.3246	1525.8278	1540.9887
1636.8325	1705.1832	1757.5947
3020.4725	3021.9059	3085.4898
3090.8631	3135.1864	3136.4074
3153.0025	3157.1694	3232.1383
3266.6685	3471.0615	3564.3648

IV. Changes in Gibbs free energy along the reaction profiles

Table S1a. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (8) of Figure 1 at different temperatures with respect to the initial reactants.

Stationary point	**From purine to adenine**			
	ts1a	***i1***	***ts1b***	***adenine+H***
	ΔE, kJ mol^{-1}			
	33	-57	54	2
Temperature, °K	***ΔG***, kJ mol^{-1}			
10	32	-57	54	2
25	31	-56	55	3
50	30	-53	58	4
100	30	-46	65	7
150	30	-39	72	10
200	30	-32	80	13
250	29	-24	87	15
298.15	27	-17	95	18

Table S1b. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (9) of Figure 2 at different temperatures with respect to the initial reactants.

Stationary point	**From purine to *1H*-purin-6(*7H*)-one**						
	i2-complex	***ts2a***	***i3***	***ts2b***	***7H-purin-6-ol+H***	***ts2c***	***1H-purin-6(7H)-one+H***
	ΔE, kJ mol^{-1}						
	-11	-6	-88	3	-43	97	-66
Temperature, °K	***ΔG***, kJ mol^{-1}						
10	-11	-6	-88	3	-43	97	-66
25	-9	-4	-86	5	-42	98	-65
50	-7	-2	-84	7	-41	99	-64
100	-2	4	-78	14	-39	101	-62
150	3	11	-71	21	-36	104	-59
200	8	17	-64	28	-34	106	-57
250	13	24	-57	35	-31	109	-54
298.15	18	31	-50	43	-29	111	-52

Table S1c. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (10) of Figure 2 at different temperatures with respect to the initial reactants.

Stationary point	**From *1H*-purin-6(*7H*)-one to guanine**			
	ts2d	***i4***	***ts2e***	***guanine+H***
	ΔE, kJ mol^{-1}			
	30	-74	56	5
Temperature, °K	***ΔG***, kJ mol^{-1}			
10	30	-74	56	5
25	32	-72	58	6
50	35	-70	61	7
100	41	-63	67	10
150	48	-56	75	13
200	55	-49	82	16
250	63	-42	90	18
298.15	70	-34	97	21

Table S1d. Relative in Gibbs free energy, ΔG, calculated for all stationary points in scheme (11) of Figure 2 at different temperatures with respect to the initial reactants.

Stationary point		**From purine to *7H*-purin-2-amine**			
		ts2f	***i5***	***ts2g***	***7H-purin-2-amine +H***
		ΔE, kJ mol^{-1}			
		47	-30	46	-3
Temperature, °K		***ΔG***, kJ mol^{-1}			
10		47	-30	46	-3
25		49	-28	48	-2
50		51	-26	51	-1
100		58	-19	57	2
150		65	-12	65	5
200		72	-5	72	8
250		79	2	80	10
298.15		86	9	88	13

Table S1e. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (12) of Figure 2 at different temperatures with respect to the initial reactants.

Stationary point	**From *7H*-purin-2-amine to guanine**						
	i6-complex	***ts2h***	***i7***	***ts2i***	***2-amino-7H-purin-6-ol+H***	***ts2j***	***guanine+H***
	ΔE, kJ mol^{-1}						
	-11	-9	-92	2	-44	97	-57
Temperature, °K	***ΔG***, kJ mol^{-1}						
10	-11	-9	-92	2	-44	97	-57
25	-9	-7	-90	4	-43	98	-56
50	-7	-5	-88	6	-42	99	-55
100	-1	1	-82	13	-40	101	-53
150	5	8	-75	20	-37	104	-50
200	10	14	-68	27	-35	106	-48
250	16	21	-61	35	-32	109	-45
298.15	22	28	-55	42	-30	111	-43

Table S1f. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (1) of Figure 3 at different temperatures with respect to the initial reactants.

Stationary point	**From pyrimidine to pyrimidin-2(*1H*)-one**					
	ts3a	***i8***	***ts3b***	***pyrimidin-2-ol+H***	***ts3c***	***pyrimidin-2(1H)-one+H***
	ΔE, kJ mol^{-1}					
	10	-71	11	-40	114	-25
Temperature, °K	***ΔG***, kJ mol^{-1}					
10	10	-71	11	-40	114	-25
25	12	-69	13	-39	115	-24
50	14	-67	15	-38	116	-23
100	20	-61	22	-36	118	-21
150	27	-54	28	-33	120	-19
200	34	-47	36	-31	123	-16
250	41	-40	43	-28	126	-14
298.15	48	-33	51	-26	128	-12

Table S1g. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (2) of Figure 3 at different temperatures with respect to the initial reactants.

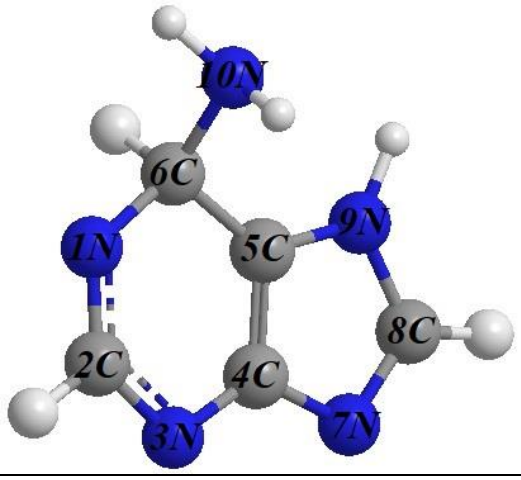
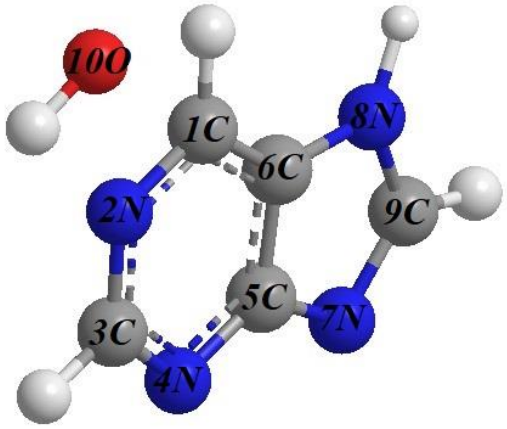
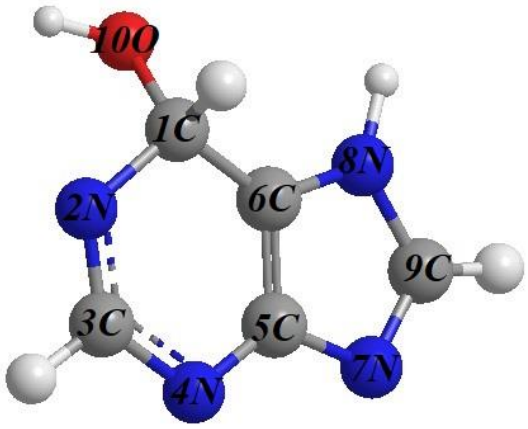
Stationary point	**From pyrimidin-2(*1H*)-one to uracil**					
	ts3d	***i9***	***ts3e***	***4-hydroxypyrimidin-2(1H)-one+H***	***ts3f***	***uracil+H***
	ΔE, kJ mol^{-1}					
	19	-59	-6	-58	68	-104
Temperature, °K	***ΔG***, kJ mol^{-1}					
10	19	-59	-6	-58	68	-104
25	21	-57	-4	-57	69	-103
50	23	-55	-2	-56	70	-102
100	29	-49	5	-54	72	-100
150	36	-42	12	-51	75	-97
200	43	-35	19	-49	77	-95
250	50	-28	26	-46	80	-92
298.15	57	-22	34	-44	83	-90

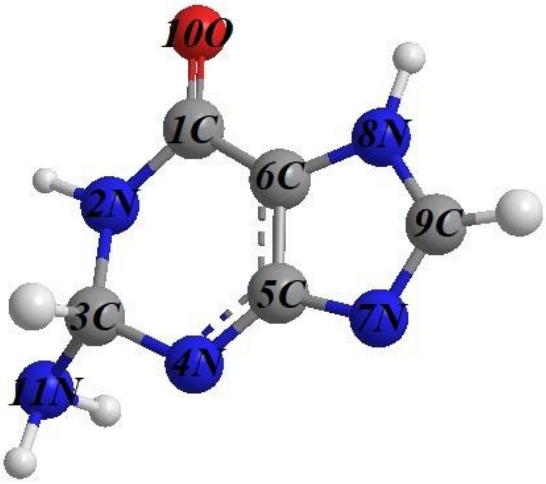
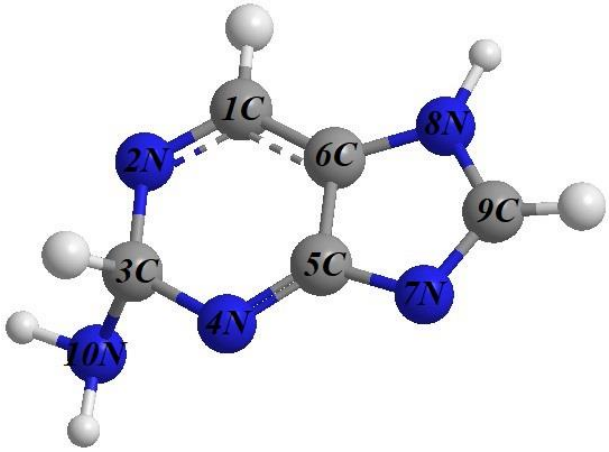
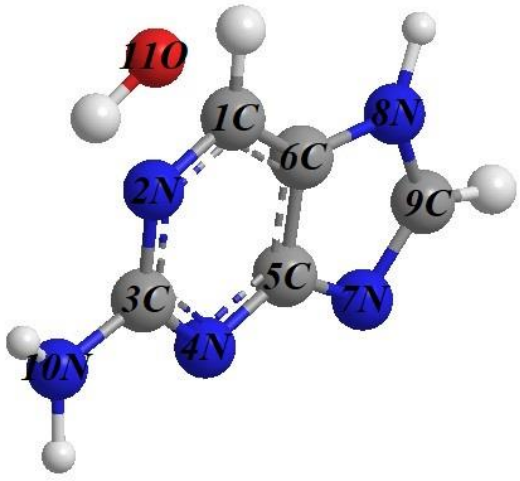
Table S1h. Relative Gibbs free energy, ΔG, calculated for all stationary points in scheme (5) of Figure 3 at different temperatures with respect to the initial reactants.

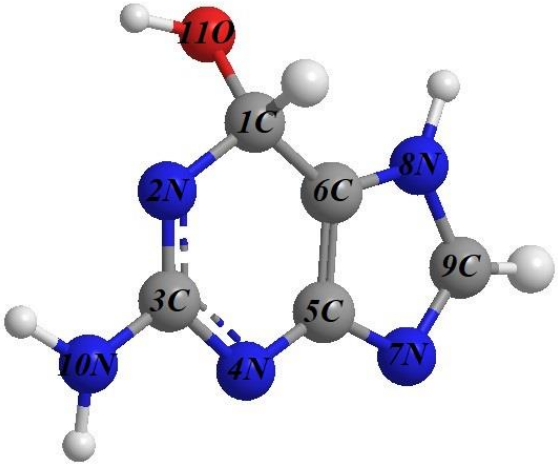
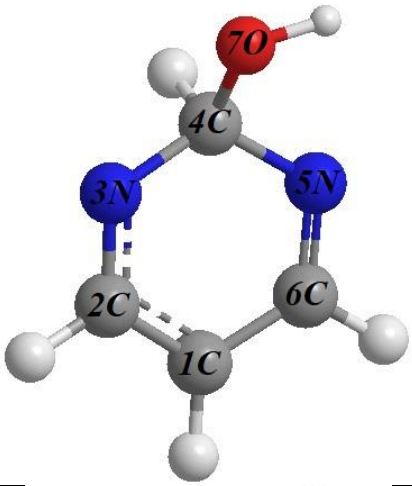
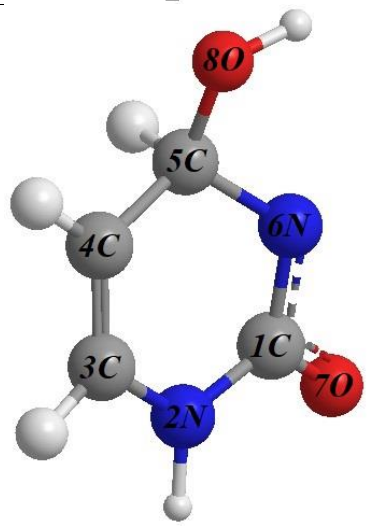
Stationary point	**From pyrimidin-2(*1H*)-one to cytosine**			
	ts3g	***i10***	***ts3h***	***cytosine+H***
	ΔE, kJ mol^{-1}			
	35	-20	39	-17
Temperature, °K	***ΔG***, kJ mol^{-1}			
10	35	-20	39	-17
25	37	-18	41	-16
50	39	-16	43	-15
100	46	-9	50	-12
150	53	-2	58	-10
200	60	5	65	-7
250	68	12	73	-5
298.15	75	19	81	-2

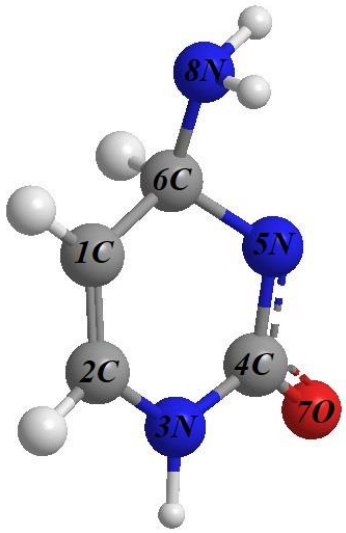
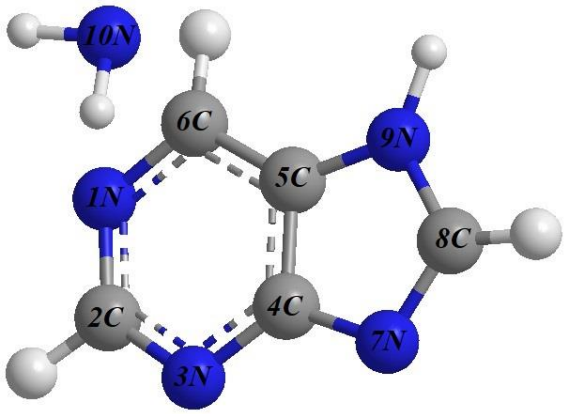
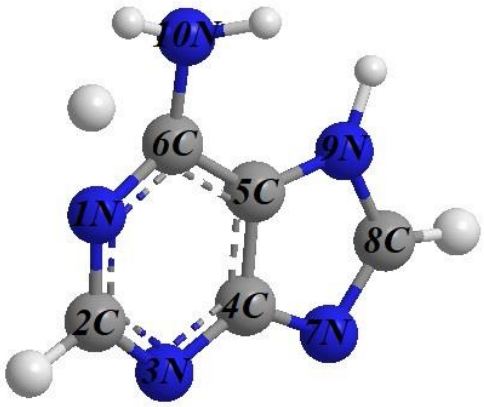
V. Spin densities

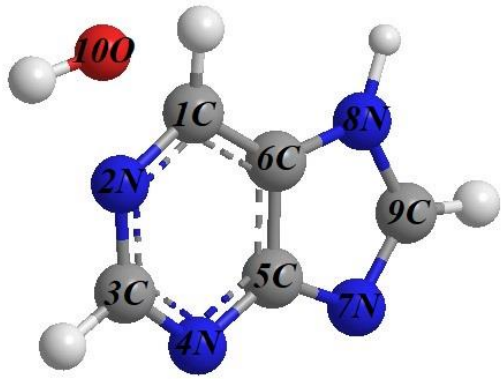
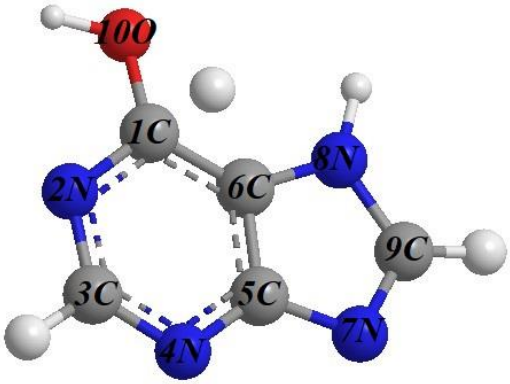
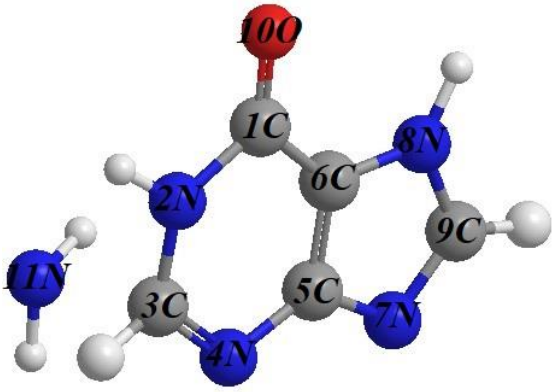
Table S2. Calculated spin densities for all doublet structures (intermediates and transition states).

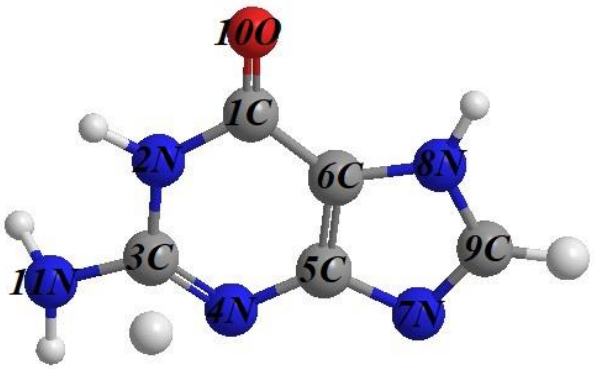
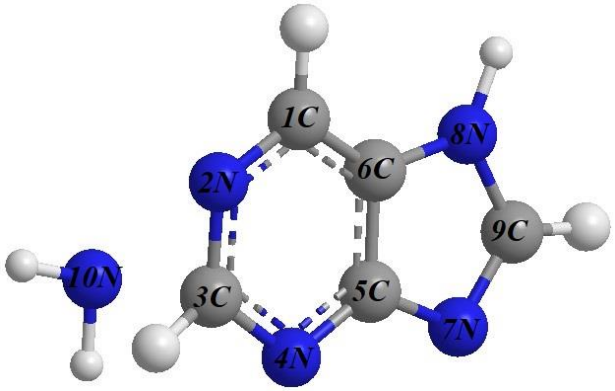
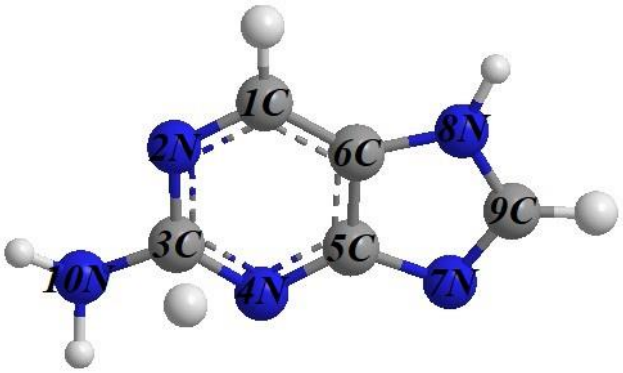
i1		1 N 0.262616 2 C -0.137870 3 N 0.473995 4 C -0.074989 5 C 0.349459 6 C -0.041431 7 N 0.022987 8 C 0.041438 9 N 0.019173 10 N 0.026039
i2-complex		1 C 0.024666 2 N -0.015167 3 C 0.024574 4 N -0.013019 5 C 0.024914 6 C 0.011462 7 N -0.007257 8 N -0.004151 9 C 0.018076 10 O 0.961559
i3		1 C -0.034334 2 N 0.253028 3 C -0.127693 4 N 0.461160 5 C -0.070236 6 C 0.357089 7 N 0.021854 8 N 0.021917 9 C 0.042740 10 O 0.021294

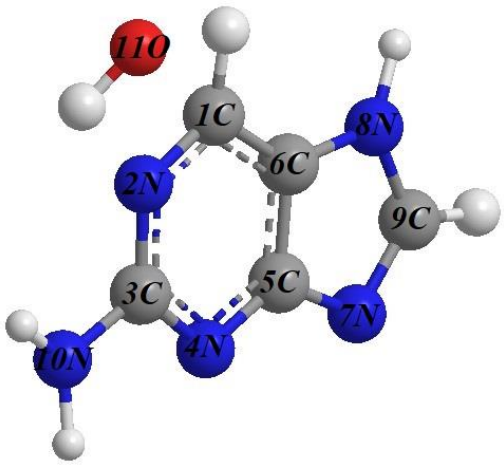
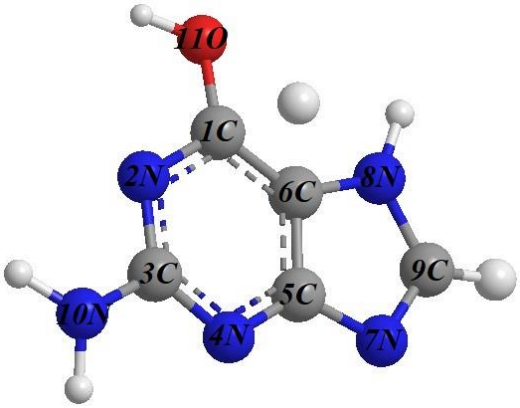
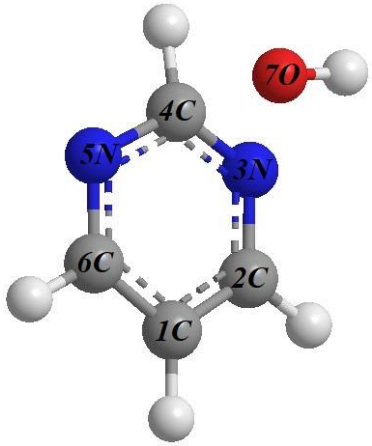
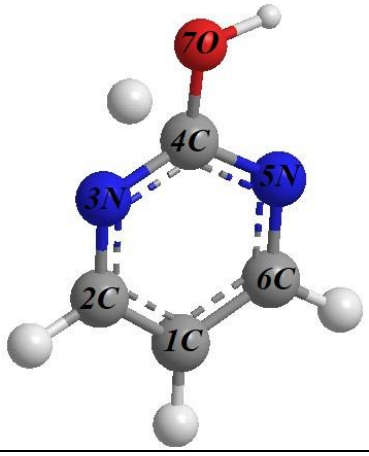
i4		1 C -0.036666 2 N 0.044362 3 C -0.033583 4 N 0.558536 5 C -0.156584 6 C 0.410963 7 N 0.074312 8 N 0.056929 9 C -0.016053 10 O 0.038190 11 N 0.017276
i5		1 C -0.158746 2 N 0.267244 3 C -0.042928 4 N 0.497647 5 C -0.165509 6 C 0.424164 7 N 0.075391 8 N 0.040809 9 C -0.026324 10 N 0.026082
i6-complex		1 C 0.035263 2 N -0.023459 3 C 0.028882 4 N -0.012044 5 C 0.043278 6 C 0.033782 7 N -0.014852 8 N -0.009597 9 C 0.038114 10 N 0.019949 11 O 0.886256

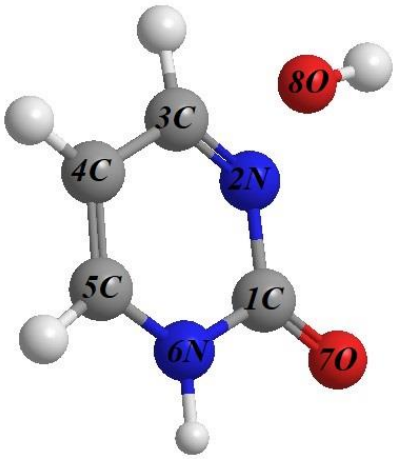
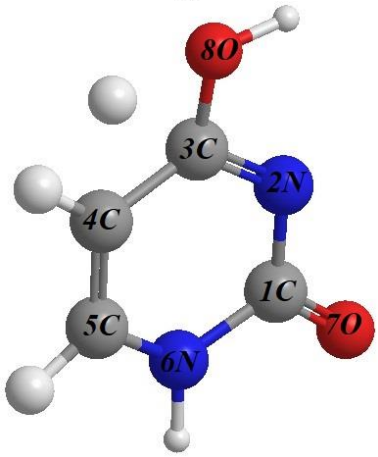
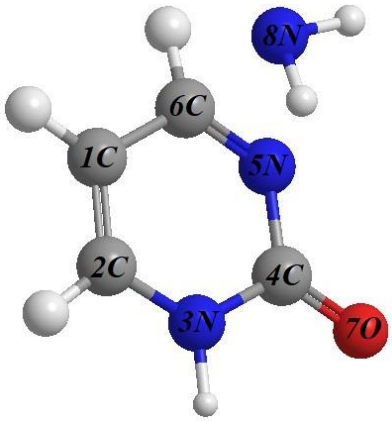
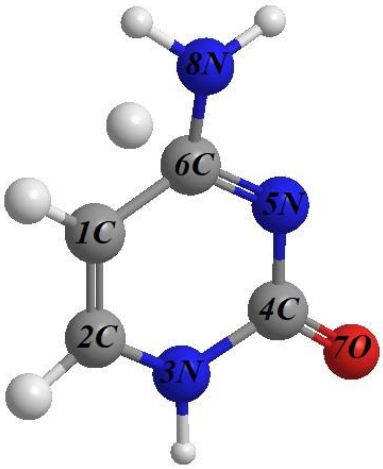
i7		1 C -0.033089 2 N 0.108611 3 C -0.053945 4 N 0.483912 5 C -0.072746 6 C 0.403470 7 N 0.024371 8 N 0.022004 9 C 0.052864 10 N 0.017511 11 O 0.019090
i8		1 C 0.645198 2 C-0.211737 3 N 0.373055 4 C -0.038402 5 N 0.365899 6 C -0.207013 7 O 0.016006
i9		1 C -0.066174 2 N 0.040547 3 C -0.017268 4 C 0.051928 5 C -0.051090 6 N 0.845655 7 O 0.102678 8 O 0.003817

i10		1 C 0.045848 2 C -0.016263 3 N 0.037394 4 C -0.065368 5 N 0.864956 6 C -0.049937 7 O 0.103784 8 N 0.004730
ts1a		1 N 0.202140 2 C -0.114333 3 N 0.201298 4 C -0.039494 5 C 0.178199 6 C -0.173070 7 N 0.006343 8 C 0.019231 9 N -0.004874 10 N 0.738301
ts1b		1 N 0.178700 2 C -0.082099 3 N 0.138366 4 C -0.013262 5 C 0.117107 6 C -0.121593 7 N -0.003931 8 C 0.033900 9 N -0.016143 10 N -0.001968

ts2a		1 C -0.140931 2 N 0.138698 3 C -0.077184 4 N 0.169866 5 C -0.024644 6 C 0.205298 7 N 0.001778 8 N -0.000481 9 C 0.028622 10 O 0.692826
ts2b		1 C -0.110831 2 N 0.167847 3 C -0.075223 4 N 0.127780 5 C -0.003995 6 C 0.118868 7 N -0.007429 8 N -0.017877 9 C 0.040506 10 O -0.006187
ts2d		1 C -0.012026 2 N 0.015100 3 C -0.153403 4 N 0.309297 5 C -0.077741 6 C 0.137023 7 N 0.037422 8 N 0.021988 9 C -0.022385 10 O 0.002653 11 N 0.772675

ts2e		1 C -0.011134 2 N 0.033159 3 C -0.134357 4 N 0.271884 5 C -0.058703 6 C 0.095762 7 N 0.028217 8 N 0.015649 9 C -0.017956 10 O -0.004190 11 N 0.003491
ts2f		1 C -0.120310 2 N 0.183789 3 C -0.186546 4 N 0.274361 5 C -0.091599 6 C 0.198987 7 N 0.036651 8 N 0.014501 9 C -0.018163 10 N 0.709572
ts2g		1 C -0.091075 2 N 0.153880 3 C -0.136022 4 N 0.240388 5 C -0.069145 6 C 0.130382 7 N 0.026189 8 N 0.006982 9 C -0.017459 10 N -0.007720

ts2h		1 C -0.079837 2 N -0.001790 3 C -0.004767 4 N 0.153550 5 C 0.032110 6 C 0.235711 7 N -0.023560 8 N -0.026636 9 C 0.087853 10 N 0.016703 11 O 0.620861
ts2i		1 C -0.098812 2 N 0.120086 3 C -0.042416 4 N 0.133496 5 C 0.012360 6 C 0.124119 7 N -0.013375 8 N -0.024767 9 C 0.059186 10 N -0.011231 11 O -0.005550
ts3a		1 C 0.281692 2 C -0.141341 3 N 0.234666 4 C -0.162910 5 N 0.204747 6 C -0.123845 7 O 0.698500
ts3b		1 C 0.179790 2 C -0.092288 3 N 0.184833 4 C -0.129367 5 N 0.183539 6 C -0.093381 7 O -0.002654

ts3d		1 C -0.036065 2 N 0.402162 3 C -0.131192 4 C 0.044533 5 C -0.054099 6 N 0.003360 7 O 0.074048 8 O 0.70229
ts3e		1 C -0.018900 2 N 0.234350 3 C -0.111496 4 C 0.042850 5 C 0.042036 6 N 0.071444 7 O 0.001328 8 O 0.005173
ts3g		1 C 0.052889 2 C -0.045512 3 N 0.024132 4 C -0.026007 5 N 0.334991 6 C -0.142913 7 O 0.046111 8 N 0.788404
ts3h		1 C 0.047060 2 C 0.013985 3 N 0.058087 4 C -0.021148 5 N 0.270796 6 C -0.121457 7 O 0.011865 8 N 0.010605

VI. Explicit solvent effects in liquid water and water ice

Table S3a. Relative energies for all the structures in sequence (1) on Figure 3 calculated at the SCRF-PCM/ωB97X-D/6-311G(d,p) level of theory using the parameters for liquid water[a] and water ice[b].

Stationary point	Water liquid	Water ice
	Relative energy, kJ mol^{-1}	
ts3a	18	20
i8	-78	-77
ts3b	9	13
pyrimidin-2-ol	-47	-43
ts3c	103	104
pyrimidin-2(*1H*)-one	-41	-49

Table S3b. Barrier heights for the H migration steps corresponding to to ***ts3c*** in sequence (1) on Figure 3 in the presence of explicit water molecules directly participating in the reaction calculated at the SCRF-PCM/ωB97X-D/6-311G(d,p) level of theory using the parameters for liquid water[a] and water ice[b]. The values for liquid water are taken from Table 1.

Stationary point	Water liquid	Water ice
	Relative energy, kJ mol^{-1}	
1 H_2O	43	46
2 H_2O	36	38
3 H_2O	48	45
4 H_2O	57	63

[a] dielectric constant 78.3553 and square of the index of refraction at optical frequencies 1.777849.
[b] dielectric constant 3.17 and square of the index of refraction at optical frequencies 1.7161.