Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information for:

Simulating the Reactions of Substituted Pyridinio-*N*-Phosphonates with Pyridine as a Model for Biological Phosphoryl Transfer

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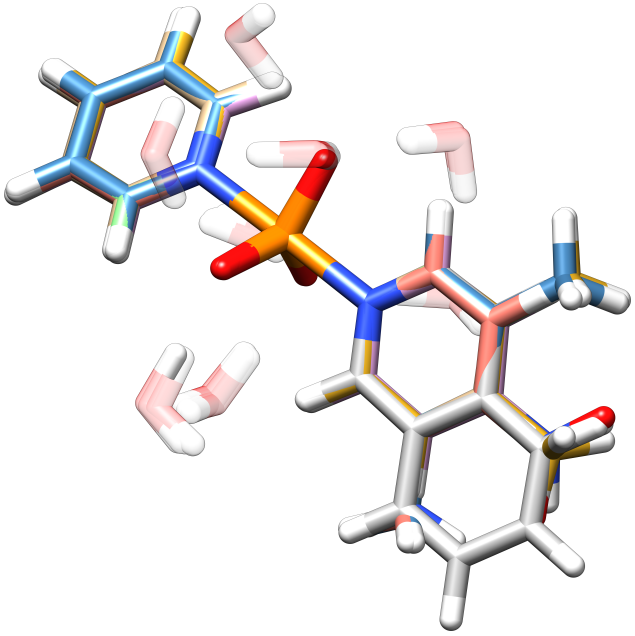

Figure S1: Overlay of transition states for the reactions of all substituted pyridinio-*N*-phosphosphonates studied in this work with pyridine, aligned to the compound with the 4-nitropyridine leaving group. For a list of compounds studied in this work see **Scheme 2** of the main text, and for details of the transition state optimization see the **Methodology** section.

Table S1: Absolute electronic energies (E_{el}, in atomic units), zero-point energy contributions (E_{ZPE}, in kcal mol^{-1}), entropies (S, in cal $mol^{-1} K^{-1}$, $-T\Delta S$ in kcal mol^{-1} calculated at 298.15K) and the lowest frequency value (ν, cm^{-1}) for stationary points obtained for the reaction of pyridine with the substituted pyridynio-*N*-phosphonates studied in this work.[a]

4NP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1879.9726	250.23	244.83	13.8	0.0	0.0	0.0	0.0
TS	-1879.9622	250.32	235.06	-135.4	6.5	0.1	2.9	9.5
PS	-1879.9873	250.97	237.83	14.7	-9.2	0.7	2.1	-6.4
PY	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1675.4886	248.51	231.45	14.4	0.0	0.0	0.0	0.0
TS	-1675.4732	248.89	218.96	-155.5	9.6	0.4	3.7	13.7
PS	-1675.4912	248.90	226.76	18.6	-1.6	0.4	1.4	0.2
IQ	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1829.1130	278.30	243.72	10.8	0.0	0.0	0.0	0.0
TS	-1829.0974	278.54	230.55	-158.6	9.8	0.2	3.9	13.9
PS	-1829.1188	278.57	237.53	20.8	-3.7	0.3	1.8	-1.6
3MP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1714.8064	266.24	236.55	20.7	0.0	0.0	0.0	0.0
TS	-1714.7904	266.39	227.02	-152.9	10.1	0.2	2.8	13.1
PS	-1714.8098	266.02	234.50	16.3	-2.1	-0.2	0.6	-1.7
3AP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1730.8568	259.14	235.28	20.0	0.0	0.0	0.0	0.0
TS	-1730.8406	259.52	223.27	-157.0	10.1	0.4	3.6	14.1
PS	-1730.8612	260.23	228.32	23.0	-2.8	1.1	2.1	0.4
35MP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1754.1237	283.40	248.72	19.7	0.0	0.0	0.0	0.0
TS	-1754.1070	283.33	239.28	-151.7	10.5	-0.1	2.8	13.2
PS	-1754.1262	284.09	242.46	15.5	-1.6	0.7	1.9	1.0
34MP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1754.1269	283.58	244.17	16.9	0.0	0.0	0.0	0.0
TS	-1754.1095	284.16	231.67	-148.4	10.9	0.6	3.7	15.2
PS	-1754.1272	283.85	239.88	18.3	-0.2	0.3	1.3	1.4
4AP	$\mathbf{E_{el}}$	$\mathbf{E_{ZPE}}$	**S**	**ν**	**ΔE**	$\mathbf{\Delta E_{ZPE}}$	**-TΔS**	**ΔG**
RS	-1730.8712	259.03	235.49	18.3	0.0	0.0	0.0	0.0
TS	-1730.8486	259.06	226.74	-153.8	14.2	0.0	2.6	16.8
PS	-1730.8677	260.07	232.29	11.0	2.2	1.0	1.0	4.2

[a] RS, TS, and PS denote the reactant, transition and product states, respectively. Relative energies (kcal mol^{-1}) are calculated with respect to reactant state. The leaving group acronyms in the table correspond to 4NP – 4-nitropyridine, PY-pyridine, IQ – isoquinoline, 3MP – 3-methylpyridine, 3AP – 3-aminopyridine, 35MP – 3,5-dimethylpyridine, 34MP – 3,4-dimethylpyridine and 4AP – 4-aminopyridine. Compounds are presented in ascending order of leaving group pK_a (see also **Table 1** of the main text).

Cartesian Coordinates of Key Stationary Points

Optimised stationary points along the reaction profiles for the reaction of pyridine with the substituted pyridynio-*N*-phosphonates (denoted by the leaving group name) calculated at the ωB97X-D/6-31+G(d) level of theory.

(a) 4-nitropyridine

RS

P	0.206361	0.434776	-0.126080
O	0.629297	-0.827436	0.616853
O	0.324303	1.729694	0.661597
O	0.552325	0.496241	-1.600919
N	-1.647493	0.189262	-0.166706
C	-2.468451	1.015765	0.500393
H	-2.012852	1.866012	0.989855
C	-3.831552	0.778642	0.554704
H	-4.481227	1.453580	1.096458
C	-4.304904	-0.343141	-0.100394
C	-3.468054	-1.202368	-0.793946
H	-3.833410	-2.081143	-1.308993
C	-2.120738	-0.899597	-0.801279
H	-1.400069	-1.528606	-1.309923
H	0.522691	-0.934280	-2.657343
O	0.510900	-1.746733	-3.213531
H	-0.410311	-1.834087	-3.495807
H	0.582052	-2.862883	-1.704535
O	0.590607	-3.248888	-0.804514
H	0.611045	-2.453347	-0.233005
H	-0.763170	0.316672	3.234833
O	-0.507047	1.254523	3.346447
H	-0.164383	1.497798	2.462864
H	-1.972088	-1.452033	2.314621
O	-1.090219	-1.487957	2.712781
H	-0.475134	-1.352284	1.958901
H	1.858493	-0.634217	1.930104
O	2.514527	-0.559818	2.655599
H	3.371949	-0.645007	2.214010
H	-0.445946	3.201159	-0.262214
O	-0.676839	3.881141	-0.925508
H	0.015734	3.743904	-1.601288
H	1.777051	2.793494	0.469321
O	2.502402	3.420006	0.255208
H	2.114854	4.293420	0.407114
O	1.614551	2.972506	-2.416082
H	2.089735	3.198276	-1.589809
H	1.261285	2.077248	-2.226339
N	-5.751826	-0.634946	-0.061245
H	5.507223	1.216226	0.170257
C	5.101238	0.213928	0.063772
C	5.590180	-0.826822	0.848690
H	6.378463	-0.639845	1.570644
C	5.044290	-2.098019	0.683045

H	5.398483	-2.935351	1.276964
C	4.029355	-2.268559	-0.254114
H	3.564951	-3.235832	-0.415044
C	3.607736	-1.163130	-0.986837
H	2.815758	-1.266285	-1.722960
N	4.129855	0.063263	-0.847163
O	-6.141224	-1.646078	-0.622706
O	-6.472952	0.151864	0.530289

TS

P	0.516685	0.162438	-0.087353
O	0.483334	-1.192770	0.622959
O	0.607800	1.447874	0.729744
O	0.653673	0.228357	-1.600761
N	-1.535527	0.197073	-0.148825
C	-2.254185	1.069423	0.563486
H	-1.700160	1.830182	1.098553
C	-3.639341	1.002523	0.623832
H	-4.200284	1.719704	1.208910
C	-4.249427	-0.016224	-0.085170
C	-3.520852	-0.929158	-0.831562
H	-3.991063	-1.729189	-1.388369
C	-2.144378	-0.783085	-0.830372
H	-1.507791	-1.467318	-1.379971
H	0.434142	-1.023457	-2.770638
O	0.345169	-1.771306	-3.409276
H	-0.602758	-1.822693	-3.595274
H	0.543043	-2.952671	-1.970733
O	0.644436	-3.400350	-1.105916
H	0.592579	-2.659027	-0.466331
H	-0.635211	0.105158	3.255604
O	-0.179192	0.960281	3.390924
H	0.141536	1.186099	2.492276
H	-2.198273	-1.383048	2.309159
O	-1.319373	-1.576024	2.666212
H	-0.713449	-1.504477	1.892542
H	1.771783	-2.114312	1.474605
O	2.385822	-2.718353	1.945803
H	3.228501	-2.615229	1.481187
H	-0.113255	2.904671	-0.330896
O	-0.321802	3.556303	-1.028685
H	0.373820	3.375610	-1.688906
H	1.983029	2.599256	0.484522
O	2.686318	3.246176	0.251748
H	2.229315	4.098943	0.235945
O	2.027327	2.503080	-2.424028
H	2.436442	2.779737	-1.578603
H	1.593453	1.650988	-2.195067
N	-5.717654	-0.135584	-0.045568
H	2.896746	0.822223	1.907273
C	3.470819	0.304213	1.144208
C	4.812426	-0.002926	1.334190
H	5.309507	0.285803	2.254072

C	5.486744	-0.691964	0.329474
H	6.534013	-0.953492	0.446728
C	4.795061	-1.042097	-0.827794
H	5.279193	-1.581322	-1.634931
C	3.455960	-0.687596	-0.935166
H	2.870576	-0.938131	-1.815029
N	2.809954	-0.024365	0.029514
O	-6.234137	-1.041457	-0.682112
O	-6.339386	0.677053	0.621772

PS

P	0.815936	0.325177	-0.218563
O	-0.222261	-0.761511	-0.482507
O	0.842613	0.880194	1.202572
O	1.029509	1.342090	-1.324929
N	-2.539051	2.494698	0.475978
C	-2.342356	1.619939	1.468737
H	-1.764322	1.968736	2.317901
C	-2.839467	0.320346	1.461555
H	-2.659086	-0.351239	2.291529
C	-3.571049	-0.058163	0.348727
C	-3.792596	0.813984	-0.704278
H	-4.359493	0.529175	-1.581344
C	-3.246567	2.086811	-0.584041
H	-3.395119	2.811997	-1.377656
H	-0.148815	1.825534	-2.545284
O	-0.796762	2.030162	-3.257762
H	-1.444809	2.614137	-2.840266
H	-1.511642	0.305427	-3.123957
O	-1.694872	-0.628578	-2.893996
H	-1.219808	-0.737097	-2.045047
H	-0.323437	-1.441605	2.836579
O	0.051001	-0.696201	3.350324
H	0.352693	-0.087283	2.642730
H	-1.852156	-2.537762	1.535171
O	-0.885109	-2.600937	1.483874
H	-0.641487	-1.960888	0.777190
H	0.394451	-2.306968	-1.354777
O	0.705950	-3.123250	-1.796477
H	1.666002	-3.017385	-1.855811
H	0.797010	2.743937	1.363555
O	0.988275	3.703904	1.343473
H	1.744909	3.745162	0.728537
H	2.541341	1.257648	1.774815
O	3.486558	1.492330	1.901394
H	3.471136	2.233942	2.522690
O	3.154208	3.027705	-0.492475
H	3.441500	2.485882	0.271699
H	2.447299	2.483800	-0.899455
N	-4.132267	-1.412673	0.281333
H	1.808578	-1.655359	1.461683
C	2.578341	-1.572586	0.702750
C	3.707542	-2.365025	0.704813

H	3.837846	-3.102099	1.488063
C	4.652838	-2.196135	-0.305374
H	5.548038	-2.808764	-0.324708
C	4.438106	-1.234491	-1.288135
H	5.149029	-1.072547	-2.089443
C	3.287076	-0.469772	-1.240497
H	3.053767	0.291395	-1.974176
N	2.384663	-0.644322	-0.257444
O	-4.883525	-1.682044	-0.643139
O	-3.825218	-2.212463	1.158849

(b) Pyridine

RS

P	-0.466785	0.419661	-0.132195
O	-0.045403	-0.846914	0.610683
O	-0.239660	1.719844	0.628288
O	-0.160408	0.445986	-1.619891
N	-2.305509	0.263304	-0.094305
C	-3.073133	1.170644	0.538581
H	-2.558396	2.017124	0.973327
C	-4.444049	1.007993	0.617929
H	-5.036367	1.755148	1.132491
C	-5.027797	-0.114069	0.038308
C	-4.219050	-1.046333	-0.609961
C	-2.856937	-0.833053	-0.656760
H	-2.178258	-1.528466	-1.136230
H	-0.345602	-0.982624	-2.648063
O	-0.438893	-1.799950	-3.190969
H	-1.382419	-1.845149	-3.399992
H	-0.297735	-2.903847	-1.673324
O	-0.239692	-3.282619	-0.772185
H	-0.157092	-2.482574	-0.211866
H	-1.304930	0.412030	3.257993
O	-1.024765	1.346178	3.337671
H	-0.697163	1.556322	2.439515
H	-2.593029	-1.321543	2.405183
O	-1.701689	-1.391976	2.777010
H	-1.105609	-1.293891	2.001041
H	1.249150	-0.634374	1.849579
O	1.941292	-0.544367	2.539763
H	2.776163	-0.577390	2.050807
H	-0.921069	3.209411	-0.309327
O	-1.103470	3.906657	-0.971003
H	-0.428410	3.715378	-1.651582
H	1.281683	2.657264	0.394935
O	2.063816	3.205264	0.162706
H	1.772064	4.115177	0.313950
O	1.085294	2.810993	-2.485814
H	1.597424	3.005633	-1.673901
H	0.662635	1.950686	-2.274471
H	-6.101108	-0.262894	0.091128
H	4.921302	0.912878	-0.156819

C	4.455741	-0.068117	-0.197800
C	4.923573	-1.099913	0.611166
H	5.755175	-0.926876	1.286502
C	4.300943	-2.343717	0.529570
H	4.636997	-3.173542	1.144201
C	3.233189	-2.495786	-0.349876
H	2.708075	-3.440601	-0.443481
C	2.838857	-1.401274	-1.113866
H	2.007477	-1.490137	-1.807446
N	3.435138	-0.202657	-1.056326
H	-4.633454	-1.934531	-1.071883

TS

P	0.578361	0.158810	-0.085468
O	0.473956	-1.198881	0.626518
O	0.612859	1.458143	0.724336
O	0.667572	0.225405	-1.607708
N	-1.535563	0.207362	-0.154166
C	-2.263729	1.057928	0.577622
H	-1.708907	1.805406	1.132696
C	-3.649579	0.984285	0.631029
H	-4.201716	1.693583	1.237537
C	-4.296340	-0.009906	-0.095747
C	-3.532661	-0.894403	-0.855199
C	-2.154168	-0.754210	-0.854680
H	-1.515983	-1.425176	-1.420942
H	0.489322	-1.057184	-2.739384
O	0.431803	-1.813291	-3.373669
H	-0.513114	-1.906516	-3.558500
H	0.688578	-2.984752	-1.932120
O	0.798504	-3.409281	-1.056787
H	0.695602	-2.657892	-0.433886
H	-0.522593	0.123172	3.284109
O	-0.049215	0.972057	3.396457
H	0.227284	1.193705	2.480633
H	-2.167901	-1.267483	2.382592
O	-1.286237	-1.524190	2.688720
H	-0.710579	-1.443854	1.890682
H	1.700265	-2.066934	1.585470
O	2.299876	-2.636539	2.117082
H	3.159461	-2.554374	1.680458
H	-0.144208	2.867243	-0.337154
O	-0.355170	3.530940	-1.024321
H	0.350715	3.373802	-1.679600
H	1.950444	2.635090	0.487265
O	2.661611	3.275548	0.256208
H	2.210386	4.130811	0.221933
O	2.007728	2.513954	-2.421972
H	2.416295	2.789698	-1.576127
H	1.578632	1.657434	-2.196090
H	-5.378069	-0.096760	-0.071253
H	2.744568	0.822926	1.931841
C	3.344629	0.331067	1.173333

C	4.694511	0.074877	1.366242
H	5.173812	0.379594	2.290061
C	5.401035	-0.581015	0.361795
H	6.457175	-0.800648	0.483673
C	4.730797	-0.952613	-0.800985
H	5.239802	-1.467513	-1.608318
C	3.380704	-0.653918	-0.917319
H	2.808942	-0.918906	-1.800259
N	2.706540	-0.020591	0.050296
H	-3.993149	-1.685724	-1.436270

PS

P	0.281565	0.020188	-0.398533
O	-0.493085	-1.052337	0.362440
O	0.077198	1.451719	0.088126
O	0.379317	-0.154102	-1.902967
N	-3.422901	0.818810	-1.184528
C	-3.234581	1.474875	-0.030580
H	-2.878522	2.498052	-0.112876
C	-3.473716	0.916584	1.221145
H	-3.302499	1.501590	2.118759
C	-3.928902	-0.397082	1.288146
C	-4.117285	-1.096608	0.100232
C	-3.849322	-0.449065	-1.102031
H	-3.994086	-0.969947	-2.044701
H	-0.740107	-1.005527	-2.967718
O	-1.334180	-1.555288	-3.527935
H	-2.162921	-1.058189	-3.566369
H	-1.596330	-2.717511	-2.075928
O	-1.583212	-3.157475	-1.201436
H	-1.239364	-2.455535	-0.611900
H	-0.625509	1.080083	3.039351
O	-0.426364	2.001044	2.771729
H	-0.247663	1.900840	1.812726
H	-1.836742	-0.863630	3.237691
O	-0.884705	-0.774934	3.091376
H	-0.771312	-0.882176	2.119076
H	0.506050	-2.537896	0.946976
O	1.000382	-3.324832	1.254383
H	1.871508	-2.984471	1.502517
H	-0.434841	2.669854	-1.241946
O	-0.483341	3.263134	-2.019243
H	0.302873	2.992131	-2.529213
H	1.563447	2.490258	-0.030170
O	2.404348	2.954393	-0.237755
H	2.142005	3.872247	-0.395149
O	1.989433	1.953417	-2.888242
H	2.300755	2.293557	-2.024087
H	1.469976	1.158773	-2.642783
H	-4.127521	-0.867529	2.247078
H	1.550247	0.361969	2.061216
C	2.329521	-0.063732	1.439643
C	3.590006	-0.345712	1.925202

H	3.817286	-0.138946	2.964142
C	4.539694	-0.892136	1.063514
H	5.536864	-1.122708	1.423365
C	4.197193	-1.136754	-0.262879
H	4.906636	-1.558637	-0.964657
C	2.918177	-0.836009	-0.693570
H	2.584002	-1.005133	-1.709345
N	2.012576	-0.308163	0.150753
H	-4.462090	-2.125435	0.097834

(c) Isoquinoline

RS

P	0.268345	0.532700	-0.125215
O	0.609098	-0.650908	0.779476
O	0.607235	1.901082	0.452347
O	0.553647	0.335884	-1.604762
N	-1.574353	0.521602	-0.052096
C	-2.271019	1.583724	0.465837
H	-1.679263	2.440582	0.755588
C	-3.625755	1.535753	0.598475
H	-4.151774	2.390007	1.010888
C	-3.596682	-0.713675	-0.326883
C	-2.204491	-0.584860	-0.429504
H	-1.599118	-1.398369	-0.816181
H	0.221061	-1.210637	-2.405599
O	0.049454	-2.087696	-2.821289
H	-0.903105	-2.094453	-2.990202
H	0.167099	-2.990164	-1.176006
O	0.225180	-3.240662	-0.231103
H	0.370478	-2.375639	0.206588
H	-0.500035	1.046378	3.244354
O	-0.150378	1.959126	3.196734
H	0.168244	2.025095	2.273550
H	-1.942324	-0.654037	2.653350
O	-1.049909	-0.766882	3.011767
H	-0.471113	-0.819722	2.218508
H	1.922553	-0.362081	1.974357
O	2.624495	-0.227573	2.647529
H	3.451690	-0.331993	2.155791
H	0.049610	3.315205	-0.641570
O	-0.097487	3.950202	-1.371770
H	0.524980	3.619989	-2.048902
H	2.213396	2.634410	0.080254
O	3.037886	3.068718	-0.232463
H	2.847069	4.015147	-0.171066
O	1.923670	2.480890	-2.797162
H	2.481057	2.721956	-2.028806
H	1.438159	1.692595	-2.470890
H	5.612481	0.706348	-0.420540
C	5.102368	-0.240037	-0.262665
C	5.538383	-1.114158	0.729382
H	6.389124	-0.851919	1.349998

C	4.858571	-2.318163	0.900383
H	5.167553	-3.025618	1.664115
C	3.769169	-2.589415	0.077620
H	3.200132	-3.507796	0.177469
C	3.411037	-1.649133	-0.883788
H	2.563915	-1.832652	-1.538785
N	4.062351	-0.492837	-1.069145
H	-6.319911	1.081041	0.724442
C	-5.746650	0.252810	0.318919
C	-6.364262	-0.906917	-0.082921
C	-5.619153	-1.992271	-0.613307
H	-3.669723	-2.723432	-1.138433
C	-4.257123	-1.903394	-0.735797
C	-4.340442	0.375662	0.205216
H	-7.442507	-1.000416	0.005294
H	-6.137742	-2.894694	-0.920867

TS

P	0.575129	0.156074	-0.086772
O	0.481259	-1.201425	0.626647
O	0.610155	1.455137	0.723250
O	0.671427	0.224141	-1.608630
N	-1.533309	0.202477	-0.160462
C	-2.274437	1.069627	0.585798
H	-1.710331	1.805533	1.144960
C	-3.639421	1.009795	0.629480
H	-4.194502	1.718196	1.236266
C	-3.541579	-0.882701	-0.887926
C	-2.138687	-0.735201	-0.859729
H	-1.508312	-1.416318	-1.425237
H	0.444796	-1.028280	-2.766957
O	0.342605	-1.774068	-3.407481
H	-0.605752	-1.804039	-3.596593
H	0.507139	-2.964772	-1.965786
O	0.587644	-3.406913	-1.096186
H	0.550923	-2.658698	-0.462289
H	-0.518218	0.138263	3.286114
O	-0.044223	0.987162	3.396730
H	0.230090	1.206291	2.479603
H	-2.155241	-1.240667	2.390743
O	-1.277952	-1.510036	2.698644
H	-0.701165	-1.441198	1.900629
H	1.746212	-2.130650	1.486247
O	2.357679	-2.724600	1.975626
H	3.217700	-2.587392	1.553777
H	-0.156951	2.857506	-0.343660
O	-0.363026	3.518565	-1.034860
H	0.347220	3.360693	-1.684591
H	1.936563	2.638109	0.491996
O	2.641676	3.287254	0.265728
H	2.179990	4.136652	0.225170
O	2.036456	2.505479	-2.415591
H	2.422128	2.790437	-1.562072

H	1.603748	1.650359	-2.193231
H	2.757508	0.840708	1.922511
C	3.353952	0.338045	1.168159
C	4.702067	0.073659	1.363837
H	5.183442	0.383301	2.284912
C	5.403439	-0.597869	0.366120
H	6.457774	-0.824598	0.490322
C	4.730248	-0.975894	-0.792988
H	5.235565	-1.503079	-1.594718
C	3.382446	-0.667603	-0.912288
H	2.808169	-0.939060	-1.791762
N	2.713295	-0.019024	0.048500
H	-6.339471	0.570635	0.456557
C	-5.736814	-0.116268	-0.130886
C	-6.323745	-1.105314	-0.881902
C	-5.538473	-2.003768	-1.650383
H	-3.555897	-2.578095	-2.238938
C	-4.170891	-1.897913	-1.655938
C	-4.324226	0.017595	-0.117344
H	-7.405136	-1.205907	-0.891308
H	-6.029331	-2.776206	-2.234411

PS

P	0.829432	0.300077	-0.325539
O	-0.060383	-0.843920	-0.804147
O	0.496250	0.867415	1.050404
O	1.247278	1.317732	-1.371642
N	-2.416521	2.382517	-0.499726
C	-2.552963	2.435313	0.858483
H	-2.262233	3.372297	1.323066
C	-3.026439	1.400085	1.618658
H	-3.111718	1.502254	2.696602
C	-3.265549	0.119848	-0.424245
C	-2.749599	1.258822	-1.097361
H	-2.631295	1.217872	-2.178567
H	0.299726	1.842783	-2.767891
O	-0.188310	2.041059	-3.599579
H	-0.979207	2.518334	-3.312424
H	-0.728121	0.243092	-3.677247
O	-0.888800	-0.708353	-3.512271
H	-0.637405	-0.810624	-2.571510
H	-0.736886	-1.529764	2.491920
O	-0.535123	-0.761083	3.064354
H	-0.179303	-0.114826	2.418444
H	-1.887311	-2.741233	0.969180
O	-0.922575	-2.713306	1.051099
H	-0.640178	-2.048532	0.382049
H	0.799433	-2.356657	-1.491446
O	1.246426	-3.153707	-1.843249
H	2.043089	-3.243281	-1.301371
H	0.413119	2.782101	1.126785
O	0.632239	3.735363	1.120267
H	1.518633	3.738625	0.712409

H	1.980715	1.320413	2.035868
O	2.852569	1.590339	2.397591
H	2.660815	2.378434	2.925247
O	3.173805	2.972441	-0.097205
H	3.246580	2.458575	0.733210
H	2.567957	2.432397	-0.646724
H	1.590294	-1.487548	1.686723
C	2.468114	-1.440422	1.052562
C	3.595944	-2.197510	1.295760
H	3.612182	-2.867521	2.147042
C	4.686961	-2.079828	0.436571
H	5.584164	-2.665434	0.607753
C	4.614768	-1.203053	-0.641717
H	5.440827	-1.082544	-1.332384
C	3.458046	-0.471486	-0.837103
H	3.332529	0.222805	-1.658319
N	2.413473	-0.593862	0.003271
H	-4.051847	-0.875031	2.760043
C	-3.941609	-0.927060	1.680275
C	-4.310894	-2.055520	0.987778
C	-4.158308	-2.126062	-0.421747
H	-3.515613	-1.104100	-2.194741
C	-3.640742	-1.060452	-1.116192
C	-3.412230	0.191308	0.984002
H	-4.719018	-2.909245	1.521232
H	-4.450087	-3.031117	-0.946000

(d) 3-methylpyridine

RS

P	-0.322222	0.462064	-0.090107
O	0.161839	-0.728274	0.736436
O	-0.158031	1.820290	0.580348
O	-0.014046	0.401224	-1.576971
N	-2.148461	0.217423	-0.035863
C	-2.961673	1.131389	0.520482
H	-2.496817	2.039214	0.880869
C	-4.320800	0.891291	0.616394
H	-4.960543	1.640218	1.067995
C	-4.833706	-0.306768	0.137501
C	-3.984764	-1.258959	-0.440178
C	-4.502777	-2.565629	-0.967742
C	-2.637416	-0.952216	-0.502323
H	-1.916526	-1.644057	-0.923185
H	-0.128162	-1.121749	-2.477108
O	-0.178730	-1.980046	-2.959090
H	-1.120520	-2.097026	-3.147446
H	0.028136	-2.975488	-1.371751
O	0.109438	-3.270569	-0.441734
H	0.146830	-2.420412	0.045480
H	-1.191195	0.579183	3.269437
O	-0.945441	1.525650	3.304493
H	-0.625531	1.707091	2.397326

H	-2.391166	-1.274207	2.524807
O	-1.498491	-1.268056	2.899718
H	-0.905342	-1.175441	2.120895
H	1.436180	-0.397181	1.959049
O	2.119792	-0.243093	2.646793
H	2.959662	-0.303553	2.169712
H	-0.901064	3.211888	-0.456283
O	-1.127629	3.851940	-1.160689
H	-0.460731	3.640662	-1.843070
H	1.319819	2.811467	0.265054
O	2.064182	3.388420	-0.015952
H	1.715805	4.286653	0.072880
O	1.094625	2.753776	-2.624659
H	1.599122	3.036398	-1.834417
H	0.716968	1.892522	-2.342680
H	-5.898162	-0.511163	0.210707
H	5.053438	1.243544	-0.245056
C	4.642635	0.239170	-0.187952
C	5.191778	-0.693466	0.687571
H	6.032350	-0.419604	1.316953
C	4.637018	-1.970723	0.732328
H	5.036606	-2.725819	1.402797
C	3.554625	-2.254645	-0.095549
H	3.081272	-3.230921	-0.092407
C	3.077568	-1.252055	-0.934705
H	2.233792	-1.444800	-1.591097
N	3.606307	-0.022286	-0.996632
H	-5.228427	-2.392637	-1.769172
H	-5.011170	-3.122866	-0.174282
H	-3.691219	-3.183252	-1.361430

TS

P	0.585505	0.154573	-0.082277
O	0.498513	-1.209652	0.620899
O	0.616077	1.449712	0.736003
O	0.647714	0.235887	-1.605756
N	-1.536554	0.188395	-0.123554
C	-2.270654	1.085615	0.539012
H	-1.725820	1.864685	1.058769
C	-3.658125	1.012975	0.564705
H	-4.225676	1.756696	1.113207
C	-4.289701	-0.020474	-0.114657
C	-3.527027	-0.966756	-0.808011
C	-4.161283	-2.105412	-1.556220
C	-2.147073	-0.814162	-0.772461
H	-1.497529	-1.526498	-1.271657
H	0.297894	-0.980810	-2.771796
O	0.139462	-1.708526	-3.421874
H	-0.821926	-1.733756	-3.529267
H	0.435369	-2.917089	-2.008791
O	0.605108	-3.370723	-1.158350
H	0.571302	-2.638656	-0.505433
H	-0.633385	0.094260	3.235548

O	-0.171910	0.945762	3.372437
H	0.140528	1.175529	2.470356
H	-2.204186	-1.332918	2.257060
O	-1.336186	-1.577049	2.609294
H	-0.722796	-1.492643	1.840186
H	1.769735	-2.157899	1.435173
O	2.402298	-2.762980	1.882787
H	3.236909	-2.628225	1.411972
H	-0.125492	2.852051	-0.345812
O	-0.340921	3.519997	-1.027638
H	0.357356	3.366090	-1.690680
H	1.952749	2.629625	0.495948
O	2.654922	3.278687	0.261407
H	2.188245	4.124846	0.209442
O	2.044310	2.495808	-2.423919
H	2.435131	2.775442	-1.571032
H	1.596417	1.649022	-2.199319
H	-5.373829	-0.098472	-0.108327
H	2.754195	0.800186	1.916745
C	3.349251	0.323571	1.144663
C	4.701022	0.066641	1.320888
H	5.187671	0.355591	2.245869
C	5.399378	-0.570895	0.299010
H	6.456756	-0.791076	0.407790
C	4.719450	-0.923452	-0.864106
H	5.222203	-1.423589	-1.684492
C	3.368073	-0.624924	-0.964048
H	2.787766	-0.876590	-1.845309
N	2.702263	-0.009333	0.020787
H	-4.857864	-1.730281	-2.313551
H	-4.729577	-2.748038	-0.875075
H	-3.405552	-2.718086	-2.056450

PS

P	0.404795	0.152552	-0.325019
O	-0.212843	-1.242330	-0.314612
O	0.109031	1.016402	0.896832
O	0.412822	0.881360	-1.656837
N	-3.478731	1.373436	-0.562526
C	-3.342677	1.822619	0.692293
H	-3.300561	2.900722	0.817813
C	-3.264653	0.980996	1.795814
H	-3.152473	1.396901	2.792015
C	-3.332170	-0.393245	1.592986
C	-3.473556	-0.891118	0.296805
C	-3.535017	-2.366179	0.011291
C	-3.535084	0.046536	-0.736943
H	-3.651668	-0.295424	-1.763304
H	-0.804099	0.749645	-2.928992
O	-1.438823	0.586966	-3.663809
H	-2.284790	0.921147	-3.334628
H	-1.479576	-1.221723	-3.180366
O	-1.364039	-2.095125	-2.753322

H	-0.984024	-1.862242	-1.881257
H	-0.386247	-1.069978	3.093381
O	-0.224559	-0.156988	3.408913
H	-0.108267	0.333178	2.567653
H	-1.564353	-2.768124	2.133147
O	-0.612016	-2.613469	2.061875
H	-0.502479	-2.129716	1.211348
H	0.905114	-2.687420	-0.666483
O	1.502906	-3.445424	-0.832669
H	2.370528	-3.041426	-0.976561
H	-0.486508	2.780196	0.497886
O	-0.542883	3.711808	0.203964
H	0.248554	3.795776	-0.361038
H	1.547047	2.036710	1.405887
O	2.369332	2.566146	1.494911
H	2.078519	3.401882	1.885951
O	1.934821	3.241851	-1.251062
H	2.263114	3.026704	-0.353528
H	1.444156	2.434437	-1.512712
H	-3.279579	-1.077091	2.436969
H	1.807339	-0.872669	1.858041
C	2.574604	-0.771192	1.099043
C	3.882444	-1.154072	1.315820
H	4.160589	-1.574124	2.274998
C	4.812764	-0.991958	0.290968
H	5.846264	-1.287703	0.437857
C	4.403305	-0.446955	-0.922421
H	5.095536	-0.304535	-1.743588
C	3.079496	-0.082042	-1.082923
H	2.692372	0.339735	-2.001694
N	2.192976	-0.243378	-0.082703
H	-4.019531	-2.903647	0.832732
H	-2.526771	-2.779964	-0.107914
H	-4.086575	-2.569841	-0.911591

(e) 3-aminopyridine

RS

P	-0.321845	0.452599	-0.100796
O	0.153985	-0.742510	0.723939
O	-0.146924	1.807356	0.574113
O	-0.010525	0.393806	-1.587060
N	-2.150787	0.219540	-0.050548
C	-2.954099	1.137366	0.512213
H	-2.485698	2.041401	0.875091
C	-4.314488	0.891829	0.610717
H	-4.953739	1.636547	1.070303
C	-4.839550	-0.296497	0.131691
C	-3.991671	-1.248284	-0.458706
N	-4.476137	-2.417997	-1.005920
C	-2.633877	-0.945115	-0.523126
H	-1.918801	-1.640263	-0.948239
H	-0.118375	-1.127952	-2.489062

O	-0.167902	-1.985788	-2.972061
H	-1.107656	-2.096014	-3.173959
H	0.022384	-2.985262	-1.386816
O	0.093830	-3.282009	-0.456436
H	0.133205	-2.432543	0.031976
H	-1.194836	0.570486	3.258297
O	-0.937345	1.513589	3.297854
H	-0.616793	1.695354	2.390941
H	-2.412986	-1.267193	2.497446
O	-1.522423	-1.273585	2.877563
H	-0.923901	-1.183157	2.102569
H	1.413254	-0.408720	1.962392
O	2.092417	-0.254019	2.654449
H	2.935279	-0.324012	2.183513
H	-0.862508	3.213613	-0.444763
O	-1.073548	3.870712	-1.138643
H	-0.410683	3.655194	-1.823649
H	1.361989	2.757103	0.276247
O	2.138496	3.292681	0.000015
H	1.852207	4.209401	0.115889
O	1.124862	2.745463	-2.613071
H	1.641640	3.002207	-1.821832
H	0.731629	1.887277	-2.343240
H	-5.903402	-0.501097	0.209251
H	4.952825	1.269589	-0.281683
C	4.569168	0.256055	-0.202333
C	5.114846	-0.629348	0.723345
H	5.925223	-0.309261	1.370268
C	4.595936	-1.920459	0.794204
H	4.994373	-2.639968	1.503356
C	3.549379	-2.264460	-0.056809
H	3.103841	-3.253479	-0.033520
C	3.072605	-1.305912	-0.945841
H	2.255667	-1.544805	-1.620913
N	3.569964	-0.064871	-1.035366
H	-5.356605	-2.739807	-0.621309
H	-3.800014	-3.166922	-1.101210

TS

P	0.584533	0.154675	-0.082956
O	0.498611	-1.208551	0.621353
O	0.615420	1.449475	0.734874
O	0.651413	0.235422	-1.605912
N	-1.541197	0.187674	-0.126845
C	-2.269152	1.085937	0.543132
H	-1.723744	1.866787	1.057916
C	-3.656014	0.998389	0.580124
H	-4.226293	1.735500	1.135019
C	-4.294982	-0.035933	-0.086892
C	-3.529619	-0.976827	-0.789422
N	-4.115129	-1.998725	-1.523567
C	-2.142164	-0.817535	-0.771314
H	-1.497330	-1.529008	-1.278534

H	0.330604	-0.984511	-2.770899
O	0.182275	-1.714614	-3.420804
H	-0.776801	-1.735706	-3.546790
H	0.453518	-2.918186	-2.004784
O	0.609102	-3.373894	-1.152532
H	0.574066	-2.641946	-0.499661
H	-0.630288	0.091500	3.237390
O	-0.163516	0.940014	3.374203
H	0.144270	1.171315	2.470913
H	-2.206795	-1.317203	2.248752
O	-1.344034	-1.576280	2.603565
H	-0.726202	-1.492258	1.838030
H	1.767183	-2.156535	1.440814
O	2.398552	-2.761680	1.889903
H	3.234584	-2.626137	1.421820
H	-0.125931	2.852524	-0.350141
O	-0.335840	3.519906	-1.034142
H	0.365547	3.362947	-1.693309
H	1.953119	2.628167	0.495866
O	2.655363	3.277752	0.262978
H	2.187850	4.123336	0.209134
O	2.049234	2.493284	-2.423092
H	2.440818	2.773577	-1.570809
H	1.601454	1.646605	-2.197542
H	-5.377726	-0.125163	-0.066971
H	2.753366	0.794323	1.922355
C	3.350532	0.321155	1.149728
C	4.702231	0.065093	1.328110
H	5.186600	0.351114	2.255210
C	5.403599	-0.567790	0.305337
H	6.461048	-0.786984	0.415537
C	4.726583	-0.916891	-0.860514
H	5.231752	-1.413293	-1.681691
C	3.374912	-0.619785	-0.962020
H	2.796789	-0.868795	-1.845518
N	2.706265	-0.008499	0.023416
H	-5.031919	-2.278425	-1.194239
H	-3.516269	-2.801452	-1.681488

PS

P	0.378759	0.083253	-0.316202
O	-0.168905	-1.330028	-0.135392
O	0.062678	1.066183	0.805986
O	0.330535	0.656177	-1.721044
N	-3.418645	1.408304	-0.653399
C	-3.382900	1.900455	0.593076
H	-3.370910	2.981785	0.689714
C	-3.365994	1.085156	1.719841
H	-3.330691	1.526619	2.710979
C	-3.384873	-0.294988	1.561003
C	-3.420116	-0.827255	0.268780
N	-3.496696	-2.197143	0.025326
C	-3.430740	0.081419	-0.800250

H	-3.465268	-0.297497	-1.818910
H	-0.770323	0.203795	-3.029007
O	-1.328260	-0.120585	-3.772481
H	-2.171822	0.340991	-3.668588
H	-1.545860	-1.770971	-2.912461
O	-1.472159	-2.536718	-2.306100
H	-0.970993	-2.164719	-1.549879
H	-0.355204	-0.763505	3.227583
O	-0.224318	0.184872	3.433407
H	-0.122134	0.575875	2.539731
H	-1.534789	-2.525613	2.476392
O	-0.579764	-2.414337	2.371232
H	-0.468848	-2.030858	1.470871
H	1.004357	-2.756539	-0.339345
O	1.625327	-3.508632	-0.431549
H	2.496386	-3.095261	-0.515165
H	-0.549283	2.802050	0.243320
O	-0.597581	3.707930	-0.122192
H	0.178724	3.730624	-0.713933
H	1.486518	2.174990	1.190670
O	2.305975	2.715218	1.205522
H	2.013485	3.592525	1.489648
O	1.820224	3.087199	-1.591809
H	2.167680	2.956696	-0.684905
H	1.335146	2.255008	-1.771611
H	-3.368076	-0.956328	2.423996
H	1.859397	-0.618181	1.942314
C	2.610278	-0.572011	1.161278
C	3.938226	-0.865067	1.394922
H	4.250982	-1.153117	2.391414
C	4.843821	-0.784972	0.338606
H	5.892646	-1.012270	0.498314
C	4.389905	-0.412148	-0.923007
H	5.061422	-0.340302	-1.770217
C	3.047718	-0.130433	-1.098182
H	2.626501	0.158402	-2.052850
N	2.186143	-0.207114	-0.066752
H	-3.156642	-2.760599	0.797142
H	-3.031357	-2.469896	-0.839449

(f) 3,5-dimethylpyridine

RS

P	-0.132753	0.325675	-0.186028
O	0.389529	-0.745747	0.770866
O	-0.074128	1.750561	0.351321
O	0.240068	0.143451	-1.648028
N	-1.938904	-0.031125	-0.170154
C	-2.825115	0.874334	0.280120
H	-2.423596	1.837270	0.568362
C	-4.177056	0.575338	0.369626
C	-5.157925	1.596415	0.870959
C	-4.581427	-0.701772	-0.018133

C	-3.662744	-1.645802	-0.484316
C	-4.087418	-3.023314	-0.905185
C	-2.333465	-1.265415	-0.541918
H	-1.557166	-1.943512	-0.877299
H	0.246220	-1.444756	-2.425900
O	0.258680	-2.345467	-2.826180
H	-0.669322	-2.535006	-3.023808
H	0.490113	-3.166138	-1.149276
O	0.567921	-3.375523	-0.195857
H	0.525727	-2.488037	0.218624
H	-1.132083	0.789493	3.126671
O	-0.945863	1.747677	3.058214
H	-0.605239	1.841604	2.145201
H	-2.203447	-1.178912	2.536768
O	-1.325980	-1.097698	2.938221
H	-0.708448	-1.065779	2.173421
H	1.559696	-0.181750	2.016973
O	2.198010	0.094668	2.709764
H	3.060167	0.051373	2.271584
H	-0.870206	2.997190	-0.804203
O	-1.119837	3.571074	-1.556704
H	-0.433941	3.344402	-2.214504
H	1.356035	2.793062	-0.019823
O	2.072907	3.387314	-0.334178
H	1.670542	4.267195	-0.330720
O	1.185745	2.470394	-2.893415
H	1.660008	2.850051	-2.125579
H	0.854687	1.616002	-2.540463
H	-5.633759	-0.969806	0.045596
H	5.030475	1.582408	-0.249483
C	4.728996	0.549913	-0.094860
C	5.294202	-0.198674	0.934228
H	6.037630	0.247563	1.586817
C	4.881632	-1.519167	1.099851
H	5.298386	-2.135132	1.891194
C	3.915644	-2.027610	0.235824
H	3.552555	-3.045731	0.330054
C	3.410646	-1.197072	-0.760067
H	2.654281	-1.565328	-1.447577
N	3.807480	0.070037	-0.940935
H	-4.780571	-2.967553	-1.751005
H	-4.604461	-3.531866	-0.085141
H	-3.226442	-3.628259	-1.201626
H	-4.652282	2.519736	1.165050
H	-5.705701	1.208719	1.735851
H	-5.890831	1.835319	0.093308

TS

P	0.591876	0.154961	-0.082591
O	0.498630	-1.209007	0.621100
O	0.616178	1.450293	0.735507
O	0.651534	0.234670	-1.606589
N	-1.540803	0.188916	-0.126237

C	-2.270444	1.085084	0.542822
H	-1.717715	1.864601	1.055423
C	-3.661485	1.026999	0.597174
C	-4.449540	2.055898	1.359339
C	-4.283977	-0.020686	-0.079975
C	-3.532430	-0.965977	-0.781572
C	-4.178884	-2.107949	-1.515001
C	-2.151212	-0.814674	-0.768017
H	-1.505701	-1.525751	-1.274085
H	0.316483	-1.000248	-2.762393
O	0.172806	-1.737202	-3.405252
H	-0.788552	-1.797576	-3.497099
H	0.524198	-2.937049	-1.995554
O	0.702970	-3.378398	-1.140590
H	0.641024	-2.642394	-0.494226
H	-0.658584	0.113505	3.233389
O	-0.202430	0.968546	3.368902
H	0.117084	1.193001	2.468001
H	-2.205035	-1.328375	2.251355
O	-1.337839	-1.557475	2.615780
H	-0.717606	-1.475430	1.851745
H	1.768125	-2.135253	1.471387
O	2.396108	-2.730725	1.937928
H	3.240904	-2.589766	1.487372
H	-0.148302	2.859033	-0.329816
O	-0.360165	3.530076	-1.009508
H	0.337373	3.373379	-1.673262
H	1.939888	2.640581	0.489638
O	2.648349	3.283526	0.256423
H	2.192535	4.136206	0.216117
O	2.003745	2.518404	-2.426940
H	2.409753	2.793622	-1.579846
H	1.570177	1.664215	-2.201210
H	-5.369031	-0.104223	-0.060323
H	2.745998	0.815305	1.915916
C	3.345085	0.341904	1.145089
C	4.700509	0.103050	1.318057
H	5.186230	0.402388	2.240122
C	5.404474	-0.528487	0.296271
H	6.465207	-0.733439	0.402357
C	4.725755	-0.895187	-0.863133
H	5.232401	-1.391666	-1.683325
C	3.370276	-0.615624	-0.959961
H	2.791023	-0.877687	-1.838641
N	2.699471	-0.004014	0.024189
H	-4.917903	-1.739311	-2.234197
H	-4.701185	-2.771076	-0.816660
H	-3.435342	-2.699279	-2.057455
H	-3.788395	2.768823	1.860141
H	-5.079871	1.579077	2.117505
H	-5.109185	2.614577	0.686418

PS

P	0.493861	0.104959	-0.255713
O	-0.308302	-0.963688	0.480738
O	0.523791	1.480757	0.403062
O	0.394786	0.112479	-1.770341
N	-3.089824	0.797141	-1.575477
C	-2.822514	1.632647	-0.566753
H	-2.411467	2.601462	-0.841125
C	-3.044506	1.330418	0.778862
C	-2.732735	2.332925	1.855634
C	-3.574767	0.075038	1.065455
C	-3.846583	-0.830274	0.038373
C	-4.390018	-2.202448	0.326485
C	-3.577243	-0.411408	-1.263947
H	-3.772507	-1.081480	-2.098861
H	-0.477591	-0.945227	-2.866088
O	-0.941765	-1.580936	-3.458592
H	-1.813777	-1.188037	-3.604111
H	-1.255323	-2.685009	-1.987947
O	-1.290812	-3.104642	-1.104046
H	-0.993439	-2.385256	-0.510364
H	0.081595	0.942339	3.360440
O	0.565265	1.774557	3.178440
H	0.587943	1.780281	2.198676
H	-1.744732	-0.401304	3.285046
O	-0.824660	-0.683562	3.188174
H	-0.685995	-0.753208	2.215946
H	0.591092	-2.463091	1.187882
O	1.071091	-3.239812	1.539463
H	1.880904	-3.278411	1.011017
H	0.096894	2.913363	-0.769683
O	0.115907	3.596512	-1.470254
H	0.815520	3.260981	-2.061843
H	2.119103	2.355517	0.248161
O	2.994512	2.739123	0.021443
H	2.826672	3.687806	-0.067624
O	2.282076	2.029224	-2.663288
H	2.697950	2.227075	-1.798973
H	1.650218	1.309239	-2.453429
H	-3.771350	-0.207596	2.098841
H	2.174502	0.130101	1.993021
C	2.773462	-0.366567	1.238217
C	4.035074	-0.859551	1.503896
H	4.449713	-0.746959	2.498506
C	4.741261	-1.494845	0.484870
H	5.733696	-1.891793	0.671203
C	4.160464	-1.616098	-0.774376
H	4.675224	-2.104377	-1.593177
C	2.894997	-1.100784	-0.983081
H	2.385095	-1.162568	-1.936185
N	2.226499	-0.484937	0.010721
H	-5.328974	-2.141281	0.888004
H	-3.682607	-2.780461	0.931725

H	-4.578418	-2.756652	-0.597757
H	-1.891795	2.971681	1.567776
H	-2.483485	1.834909	2.797540
H	-3.595784	2.983710	2.042153

(g) 3,4-dimethylpyridine

RS

P	-0.065520	0.260165	-0.182299
O	0.467133	-0.901031	0.657617
O	-0.072014	1.610367	0.525188
O	0.362977	0.268546	-1.640502
N	-1.853180	-0.147438	-0.278458
C	-2.787119	0.641577	0.288951
H	-2.425337	1.556086	0.741414
C	-4.129397	0.306401	0.295407
C	-5.127476	1.222620	0.940403
C	-4.518315	-0.903662	-0.310797
C	-3.528368	-1.704249	-0.888617
H	-3.785236	-2.644842	-1.363703
C	-2.208944	-1.311716	-0.856333
H	-1.414796	-1.911861	-1.284492
H	0.503764	-1.209271	-2.598674
O	0.579565	-2.046639	-3.113299
H	-0.323017	-2.230614	-3.408846
H	0.727087	-3.063351	-1.536347
O	0.760210	-3.379983	-0.610420
H	0.665262	-2.548614	-0.098738
H	-1.133125	0.283965	3.143429
O	-0.972667	1.247905	3.194946
H	-0.620473	1.460095	2.306226
H	-2.137904	-1.633897	2.290843
O	-1.273193	-1.570322	2.721695
H	-0.641699	-1.423553	1.982081
H	1.602512	-0.438574	1.978655
O	2.225046	-0.211746	2.703167
H	3.084658	-0.135335	2.264514
H	-0.913229	2.941124	-0.498160
O	-1.170162	3.581162	-1.192544
H	-0.445775	3.471729	-1.839484
H	1.318166	2.736964	0.319170
O	2.020499	3.389732	0.102356
H	1.588727	4.248779	0.209758
O	1.222892	2.772546	-2.568646
H	1.666694	3.074284	-1.749504
H	0.932235	1.864452	-2.333824
C	-5.955041	-1.319764	-0.331794
H	5.055969	1.715982	-0.059518
C	4.791311	0.663614	-0.002543
C	5.375721	-0.154723	0.960544
H	6.096655	0.257005	1.659410
C	5.011553	-1.498903	1.000890
H	5.444507	-2.168972	1.737684

C	4.072415	-1.961192	0.083002
H	3.746668	-2.996166	0.079926
C	3.544821	-1.062216	-0.838930
H	2.809374	-1.394023	-1.566293
N	3.895444	0.229745	-0.899410
H	-4.635898	2.102323	1.363122
H	-5.665235	0.706219	1.743348
H	-5.873173	1.558415	0.211150
H	-6.342850	-1.403703	0.690109
H	-6.083327	-2.279212	-0.837654
H	-6.563506	-0.565075	-0.843602

TS

P	0.603903	0.157000	-0.085807
O	0.477516	-1.198853	0.628651
O	0.621468	1.457375	0.724912
O	0.670527	0.224185	-1.609990
N	-1.541140	0.211889	-0.156433
C	-2.273275	1.055361	0.579462
H	-1.716956	1.807532	1.128633
C	-3.659956	0.992758	0.664937
C	-4.412004	1.974511	1.517730
C	-4.320712	-0.014038	-0.060699
C	-3.543204	-0.886578	-0.825764
H	-4.009434	-1.680042	-1.401770
C	-2.165828	-0.748498	-0.847262
H	-1.538086	-1.421708	-1.422828
H	0.492168	-1.063606	-2.737344
O	0.426375	-1.822663	-3.367273
H	-0.519603	-1.905556	-3.551489
H	0.659653	-2.987110	-1.917361
O	0.765039	-3.414057	-1.042698
H	0.671193	-2.661865	-0.418832
H	-0.625023	0.126483	3.238800
O	-0.146547	0.969317	3.371857
H	0.161146	1.192832	2.466477
H	-2.227867	-1.270408	2.254872
O	-1.365631	-1.525755	2.613723
H	-0.746624	-1.449533	1.847909
H	1.688558	-2.065116	1.603403
O	2.296677	-2.626514	2.134479
H	3.153096	-2.533714	1.693758
H	-0.157102	2.851331	-0.314799
O	-0.381525	3.528183	-0.985485
H	0.309541	3.382979	-1.658176
H	1.945952	2.650474	0.477959
O	2.658458	3.287376	0.241028
H	2.215940	4.147670	0.225712
O	1.977165	2.527846	-2.434105
H	2.388270	2.807953	-1.591202
H	1.554215	1.669412	-2.203817
C	-5.814208	-0.143631	-0.012010
H	2.724642	0.827862	1.923073

C	3.328133	0.342751	1.163350
C	4.681623	0.103487	1.348336
H	5.161628	0.415283	2.269221
C	5.391047	-0.543540	0.340235
H	6.450647	-0.748846	0.456389
C	4.719750	-0.924361	-0.818875
H	5.231253	-1.432008	-1.629092
C	3.365972	-0.643483	-0.929638
H	2.792706	-0.914366	-1.809360
N	2.689762	-0.017898	0.042498
H	-3.728217	2.676485	2.003023
H	-4.985278	1.458895	2.297047
H	-5.126709	2.549610	0.917609
H	-6.155711	-0.304638	1.017273
H	-6.160079	-0.977553	-0.628123
H	-6.293704	0.775896	-0.367853

PS

P	0.697937	0.348396	-0.206205
O	-0.224811	-0.754026	-0.717638
O	0.482307	0.772794	1.243215
O	1.023883	1.471542	-1.173402
N	-2.558013	1.850315	-0.264372
C	-2.832025	1.260984	0.908474
H	-2.448912	1.764175	1.794096
C	-3.571349	0.088888	1.057740
C	-3.871383	-0.460628	2.424252
C	-4.051221	-0.535767	-0.107556
C	-3.740593	0.054938	-1.331712
H	-4.078287	-0.393905	-2.261714
C	-3.004555	1.233556	-1.363263
H	-2.776614	1.708159	-2.313806
H	0.268521	1.889973	-2.701347
O	-0.127234	2.067420	-3.585630
H	-0.914683	2.597608	-3.400500
H	-0.754225	0.303509	-3.641738
O	-0.961592	-0.636273	-3.461270
H	-0.749683	-0.724618	-2.509607
H	-0.806184	-1.661549	2.547089
O	-0.478181	-0.975037	3.163277
H	-0.119268	-0.303162	2.545313
H	-2.164803	-2.610379	0.973162
O	-1.200756	-2.673154	1.016526
H	-0.880411	-1.976819	0.398466
H	0.582502	-2.311501	-1.420326
O	0.996851	-3.126156	-1.769691
H	1.938743	-2.911717	-1.828195
H	0.275799	2.603498	1.529502
O	0.390377	3.572729	1.610209
H	1.229268	3.715937	1.134912
H	2.013926	1.182075	2.142575
O	2.896871	1.463409	2.468591
H	2.706231	2.150351	3.122690

O	2.911984	3.131055	0.140485
H	3.078024	2.559669	0.918383
H	2.307121	2.592020	-0.411373
C	-4.896628	-1.775553	-0.034077
H	1.610797	-1.626494	1.540139
C	2.447187	-1.492589	0.863640
C	3.601291	-2.243319	0.956747
H	3.683840	-2.996705	1.731024
C	4.631518	-2.013943	0.046814
H	5.546691	-2.594302	0.098438
C	4.475311	-1.033193	-0.928342
H	5.252989	-0.823843	-1.652991
C	3.297295	-0.310708	-0.972725
H	3.108819	0.463192	-1.705984
N	2.311124	-0.544489	-0.086632
H	-3.424544	0.161776	3.204617
H	-3.488061	-1.481060	2.540223
H	-4.953524	-0.502999	2.598690
H	-4.408882	-2.565525	0.548026
H	-5.113481	-2.164993	-1.032456
H	-5.849222	-1.559503	0.465472

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RS

P	0.281484	0.354519	0.125906
O	-0.251564	-0.871434	-0.622361
O	0.205024	1.659225	-0.663188
O	-0.119083	0.440153	1.592477
N	2.061970	0.025300	0.182369
C	2.961827	0.803275	-0.469282
H	2.565821	1.685490	-0.954773
C	4.292647	0.493475	-0.510574
H	4.978527	1.145590	-1.039920
C	4.762910	-0.675382	0.136291
C	3.804630	-1.477484	0.806528
H	4.104833	-2.385703	1.317415
C	2.491845	-1.105201	0.802572
H	1.734488	-1.703154	1.296303
H	-0.153461	-0.977355	2.642650
O	-0.181725	-1.786726	3.205770
H	0.737260	-1.928320	3.472727
H	-0.339964	-2.899717	1.695139
O	-0.387999	-3.276503	0.792771
H	-0.352692	-2.475333	0.227294
H	1.232440	0.210819	-3.220563
O	1.022792	1.160385	-3.329181
H	0.697045	1.416522	-2.441299
H	2.337329	-1.610480	-2.274452
O	1.458621	-1.609663	-2.681382
H	0.842450	-1.434544	-1.933998
H	-1.459873	-0.556764	-1.910573
O	-2.106980	-0.419804	-2.637183

H	-2.963611	-0.360090	-2.190254
H	1.006040	3.081361	0.247429
O	1.249379	3.777069	0.892239
H	0.543981	3.680317	1.561517
H	-1.221907	2.731107	-0.510532
O	-1.944137	3.373843	-0.328238
H	-1.540968	4.237737	-0.492869
O	-1.086764	2.952911	2.363209
H	-1.550721	3.185721	1.532901
H	-0.756365	2.046151	2.178689
N	6.057236	-1.012391	0.115845
H	-4.961111	1.495430	-0.048014
C	-4.634806	0.460463	0.007938
C	-5.198681	-0.498517	-0.829249
H	-5.966437	-0.214644	-1.541684
C	-4.754702	-1.815224	-0.726376
H	-5.170555	-2.591730	-1.361520
C	-3.759262	-2.110613	0.200442
H	-3.371487	-3.117790	0.312020
C	-3.257112	-1.079539	0.988679
H	-2.478256	-1.279422	1.718949
N	-3.684089	0.188304	0.912251
H	6.737555	-0.431558	-0.355209
H	6.385281	-1.843088	0.589518

TS

P	0.653061	0.151352	-0.086011
O	0.492833	-1.202996	0.624600
O	0.638403	1.453898	0.721759
O	0.686442	0.221977	-1.611143
N	-1.559945	0.215359	-0.147882
C	-2.302638	1.061719	0.579270
H	-1.760814	1.843719	1.100755
C	-3.675954	0.965435	0.690178
H	-4.224511	1.679899	1.296140
C	-4.349126	-0.070699	0.017120
C	-3.563675	-0.958096	-0.744972
H	-4.023468	-1.780096	-1.284842
C	-2.197577	-0.777245	-0.789883
H	-1.572424	-1.459903	-1.358684
H	0.413982	-1.035027	-2.748583
O	0.303458	-1.780967	-3.388266
H	-0.649255	-1.826321	-3.549284
H	0.523091	-2.971920	-1.952668
O	0.634327	-3.408956	-1.083891
H	0.583822	-2.658651	-0.452768
H	-0.608107	0.132216	3.237319
O	-0.141657	0.983442	3.360054
H	0.162160	1.201373	2.451562
H	-2.202448	-1.273850	2.288619
O	-1.330842	-1.528718	2.624176
H	-0.727952	-1.441818	1.846365
H	1.738579	-2.124841	1.502158

O	2.367487	-2.707767	1.983770
H	3.199077	-2.616833	1.497211
H	-0.160754	2.825539	-0.338648
O	-0.390872	3.496398	-1.013458
H	0.309245	3.361274	-1.679226
H	1.942350	2.659102	0.476183
O	2.644181	3.308057	0.238936
H	2.182793	4.158057	0.208892
O	1.984485	2.535053	-2.436651
H	2.389089	2.817504	-1.591054
H	1.569343	1.671371	-2.211841
N	-5.708087	-0.185189	0.063212
H	2.723316	0.830821	1.917655
C	3.324739	0.341256	1.159782
C	4.677079	0.098411	1.342012
H	5.159273	0.412693	2.260815
C	5.382679	-0.555795	0.336023
H	6.441683	-0.763992	0.451555
C	4.708635	-0.941290	-0.819939
H	5.216765	-1.455915	-1.627632
C	3.356362	-0.657792	-0.931434
H	2.779261	-0.932814	-1.806963
N	2.685058	-0.022926	0.039670
H	-6.195991	0.296543	0.807178
H	-6.116570	-1.068463	-0.213644

PS

P	-0.467158	0.289852	0.240790
O	0.309020	-0.934406	0.713594
O	-0.223502	0.708819	-1.206294
O	-0.615113	1.427457	1.235129
N	3.165027	1.761452	0.205654
C	3.083509	1.412000	-1.087996
H	2.804978	2.201027	-1.781256
C	3.333233	0.138444	-1.573579
H	3.246657	-0.070754	-2.635579
C	3.694872	-0.870257	-0.672027
C	3.772653	-0.526042	0.683092
H	4.035367	-1.268187	1.431109
C	3.500765	0.780303	1.058193
H	3.566980	1.056845	2.107169
H	0.432568	1.796882	2.603934
O	0.973438	1.940244	3.414087
H	1.801911	2.321197	3.091688
H	1.325807	0.099508	3.494018
O	1.358721	-0.867285	3.342865
H	1.025136	-0.952753	2.426300
H	0.647636	-1.928712	-2.509443
O	0.371379	-1.220749	-3.128700
H	0.146598	-0.488178	-2.516560
H	2.066687	-2.824580	-1.057988
O	1.095393	-2.961772	-1.021567
H	0.785956	-2.264010	-0.402185

H	-0.651996	-2.328756	1.506610
O	-1.143773	-3.075441	1.905961
H	-2.073886	-2.816747	1.840291
H	0.202767	2.529642	-1.458742
O	0.186325	3.506711	-1.515589
H	-0.617714	3.725468	-1.007458
H	-1.734780	1.329708	-2.022627
O	-2.599494	1.715351	-2.284626
H	-2.378900	2.376266	-2.955877
O	-2.280486	3.370804	0.026610
H	-2.564590	2.824109	-0.735391
H	-1.740555	2.749136	0.559250
N	3.889630	-2.177761	-1.098254
H	-1.620226	-1.644275	-1.399718
C	-2.443904	-1.343160	-0.762415
C	-3.698258	-1.909654	-0.859737
H	-3.875392	-2.684109	-1.596284
C	-4.706389	-1.469993	-0.003565
H	-5.700398	-1.900893	-0.061508
C	-4.425859	-0.473103	0.925931
H	-5.181450	-0.104044	1.609112
C	-3.149965	0.057089	0.978803
H	-2.862899	0.830872	1.679271
N	-2.187770	-0.376145	0.143462
H	4.175302	-2.269900	-2.067320
H	4.458386	-2.746985	-0.480661