

The Stability of Aryl Carbanions Derived from Pyridine N-Oxide and N-Methylpyridinium: Ylide vs. Carbene Resonance Forms and the Role of Resonance in Stabilizing Aryl Anions.

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Pyridine Oxide

G3MP2 = -322.948914

H	0	0.0013140696	0.	0.0221472595
C	0	-0.0029551818	0.	1.1068616399
C	0	1.1864935995	0.	1.8358220495
C	0	-1.1981082065	0.	1.8264342802
C	0	-1.1968639711	0.	3.2072802727
H	0	-2.1580190551	0.	1.3180682968
H	0	2.1503787234	0.	1.3350327258
C	0	1.1743757911	0.	3.2166163927
N	0	-0.0140340481	0.	3.9206755051
H	0	-2.0767616392	0.	3.8386460868
H	0	2.0492764362	0.	3.8548889501
O	0	-0.0190195371	0.	5.186531255

Pyridine Oxide *ortho* anion 3

G3MP2 = -322.341765

H	-0.0018032853	0.	-2.5373981746
C	-0.0158950131	0.	-1.4465442122
C	1.1682783525	0.	-0.6814846196
C	-1.2111902502	0.	-0.7423204524
C	-1.1747047052	0.	0.64355215
H	-2.1808518416	0.	-1.2395574252
H	2.111132799	0.	-1.2391615337
C	1.2948196596	0.	0.7190436827
N	0.0213757635	0.	1.340856236
H	-2.0521239334	0.	1.2835327348
O	-0.070098327	0.	2.6236549193

Pyridine Oxide *meta* anion 4

G3MP2 = -322.342921

H	0	0.147159611	0.	-2.4066006361
C	0	0.2192964685	0.	-1.3116624717
C	0	1.4973435164	0.	-0.6887416853
C	0	-0.9872137015	0.	-0.60575679
C	0	-0.9759447899	0.	0.7818075275
H	0	-1.957412856	0.	-1.1088114722
N	0	0.2135078054	0.	1.4546460992
H	0	-1.8461038602	0.	1.4292782976
O	0	0.2255742863	0.	2.7529319491
C	0	1.3871006348	0.	0.7039759183
H	0	2.2356665912	0.	1.3918886616

Pyridine Oxide *para* anion 5

G3MP2 = -322.340208

C	0	0.1601503059	0.	-1.7157688847
C	0	-0.9688367764	0.	-0.8555077102
C	0	-0.9554212898	0.	0.540195278
H	0	-1.9790665902	0.	-1.285515505
N	0	0.2243130046	0.	1.2278061573
H	0	-1.824372801	0.	1.1935364902
O	0	0.2526906493	0.	2.5298814999
C	0	1.3729378993	0.	0.4894518961
H	0	2.269537454	0.	1.1043023566
C	0	1.3255300876	0.	-0.9055304931
H	0	2.3160646947	0.	-1.379146823

Pyridine

G3MP2 = -247.862304

H	0	-0.0003278302	0.	0.0063420361
C	0	-0.0024137339	0.	1.0933076518
C	0	1.1926208593	0.	1.8089043014
C	0	-1.2002215163	0.	1.8043234596
C	0	-1.1506900871	0.	3.1977013255
H	0	-2.1582354047	0.	1.2922864595
H	0	2.1526014667	0.	1.3005639931
C	0	1.137730787	0.	3.2021183932
N	0	-0.0078169395	0.	3.9041069322
H	0	-2.0683144047	0.	3.7832095476
H	0	2.0531052943	0.	3.7911400458

Pyridine *ortho* anion 6

G3MP2 = -247.225897

H	0	-0.0006695457	0.	-2.5300795569
C	0	-0.0116526706	0.	-1.4351192002
C	0	1.1677226362	0.	-0.6877867166
C	0	-1.2212005092	0.	-0.7397586716
C	0	-1.1458734527	0.	0.6514898717
H	0	-2.1852293556	0.	-1.2506207018
H	0	2.1104058826	0.	-1.2482446986
C	0	1.254644364	0.	0.7434382662
N	0	-0.0020421287	0.	1.3667090036
H	0	-2.0771825113	0.	1.2345344533

Pyridine meta anion 7

G3MP2 = -247.238261

H	0	0.1423290559	0.	-2.3979811544
C	0	0.2237888973	0.	-1.3001896725
C	0	1.5087275581	0.	-0.6975575294
C	0	-0.9866548394	0.	-0.5910928961
C	0	-0.929549383	0.	0.7999776018
H	0	-1.9573200033	0.	-1.0955833131
N	0	0.22976978	0.	1.4841427382
H	0	-1.8450922392	0.	1.4004340553
C	0	1.3564011023	0.	0.7130701952
H	0	2.2603435813	0.	1.3407014869

Pyridine para anion 8

G3MP2 = -247.241474

C	0	0.1596607875	0.	-1.7052654573
C	0	-0.9695435399	0.	-0.8422631094
C	0	-0.9137736623	0.	0.5551733195
H	0	-1.9820463343	0.	-1.2719070912
N	0	0.2340605628	0.	1.2634507844
H	0	-1.8319394632	0.	1.1563588639
C	0	1.34497326	0.	0.498567112
H	0	2.2921016048	0.	1.0530042716
C	0	1.3306745015	0.	-0.8999098612
H	0	2.320384437	0.	-1.3797329502

N-Methylpyridinium

G3MP2 = -287.450512

C	-0.0001778127	0.0314268025	-0.3339599913
N	0.0016517202	-0.0009711298	1.148242654
C	1.1778211491	0.0896121241	1.8112028807
C	-1.1759555127	-0.0763464204	1.8105530571
C	-1.1983462115	-0.064127327	3.1963351353
H	-2.0712854458	-0.1446200469	1.2025166092
H	2.0742030259	0.147663961	1.2036509645
C	1.1975182492	0.104801241	3.1969995088
C	-0.001031268	0.0263427596	3.9039446402
H	-2.1536991619	-0.1293835486	3.7060590233
H	2.1522969963	0.1742323855	3.7072477917
H	-0.0018949268	0.0343372492	4.9896824933
H	0.9230978288	-0.417836208	-0.6950196883
H	-0.0734092477	1.0681835642	-0.6638000356

H -0.8507891274 -0.5433154063 -0.6955834327

N-Methylpyridinium *ortho* zwitterion 9

G3MP2 = -287.021427

C	0	-0.0220282358	0.0219086417	-2.1340950703
N	0	0.0281911386	0.02118311	-0.663204534
C	0	1.2801092278	0.0174372489	-0.0923770071
C	0	-1.1768266963	0.0243247323	-0.021512386
C	0	-1.217681477	0.0239246744	1.3536430108
H	0	-2.0701081694	0.027065693	-0.640530369
C	0	1.1818129412	0.0171710166	1.3289563884
C	0	-0.0038385245	0.0202452979	2.0505154796
H	0	-2.1761236144	0.0264346911	1.8627670031
H	0	2.1199602638	0.0143042567	1.8811664036
H	0	-0.0014649823	0.0198356591	3.1390338296
H	0	1.0110680208	0.0190344499	-2.4718006927
H	0	-0.5388920365	0.9163435848	-2.4899892321
H	0	-0.544100729	-0.8692130563	-2.4906971009

N-Methylpyridinium *meta* zwitterion 10

G3MP2 = -286.998448

C	0	0.1674361467	0.0176666917	-2.1866359143
N	0	0.1604498897	0.0480010704	-0.7197898684
C	0	-1.0279485616	0.1078838629	-0.0711400215
C	0	-1.0335854878	0.0754414755	1.3106832571
H	0	-1.9194840684	0.1769740149	-0.6858832772
C	0	1.4581559125	-0.0919342849	1.3782568287
C	0	0.1831254971	-0.036813023	1.9975099849
H	0	-1.989243742	0.131972079	1.8271592474
H	0	0.1213509426	-0.0811474896	3.0878287344
H	0	1.1356030153	0.3718271169	-2.5386571302
H	0	-0.616764909	0.6726594299	-2.5673316978
H	0	0.0009362387	-1.0018666775	-2.539838143
C	0	1.3381248333	-0.036759037	-0.0138366643
H	0	2.204545402	-0.0539052291	-0.6785332909

N-Methylpyridinium *para* zwitterion 11

G3MP2 = -286.995643

C	0	0.177851517	0.0165269818	-2.0066278018
N	0	0.1633947549	0.0542647219	-0.5427099906
C	0	-1.0159539508	0.1212166841	0.1257069873
C	0	-1.0257824148	0.0924264722	1.5112947674
H	0	-1.9047103292	0.199669604	-0.4963476598

C	0	0.1257904146	-0.0072870552	2.3423895641
H	0	-2.0159536657	0.1581369679	1.9657306255
H	0	1.1042238588	0.464548149	-2.3652275589
H	0	-0.667462279	0.5901317526	-2.3859719323
H	0	0.1088225119	-1.0150115758	-2.3579974413
C	0	1.3245288013	-0.0479248476	0.1526113362
H	0	2.2292841231	-0.0991108157	-0.4489064775
C	0	1.2984586652	-0.0755215791	1.5379902075
H	0	2.2771341687	-0.15206546	2.0150686313

N-Methylpyridinium methyl zwitterion

G3MP2 = -287.032277

C	0	-0.0827740209	0.0318037992	-2.2711082359
N	0	-0.0336859185	0.0256932859	-0.9245406913
C	0	-1.1851357139	-0.0484896374	-0.140801482
C	0	-1.1396154136	-0.0550482679	1.2335254265
H	0	-2.1113235605	-0.1001361476	-0.7021781578
H	0	-2.0878502239	-0.1153389748	1.7613718663
H	0	0.8434935138	0.0910968606	-2.8205438209
H	0	-1.0466243633	-0.022524372	-2.7521567939
C	0	1.1717987096	0.0931094	-0.2260791718
H	0	2.0546716676	0.150142836	-0.8529105735
C	0	1.2264704598	0.0871294437	1.1479167976
H	0	2.2106420123	0.1429292132	1.6058456251
C	0	0.0703520937	0.012687155	1.9293029362
H	0	0.1098349095	0.007747028	3.0123404842

Nitrobenzene

G3MP2 = -436.115529

C	0	-1.1968832888	-0.0229693799	-1.4529286237
C	0	-1.2086301912	-0.0315072779	-0.0595993907
H	0	-2.1391072273	-0.0448321633	-1.9944969935
C	0	0.0127908227	-0.0031672456	0.6057568414
H	0	-2.1326475476	-0.0592071362	0.5072878316
N	0	0.0135960023	-0.011821263	2.0757831747
O	0	1.1128681139	0.0138569885	2.6514433624
O	0	-1.0850468876	-0.0442716941	2.6523039801
C	0	1.2334909769	0.0327998222	-0.0605649905
H	0	2.1581335335	0.0537834361	0.5055907679
C	0	1.2202103601	0.0407024461	-1.4538783206
H	0	2.1618520169	0.0685681051	-1.9961839723
C	0	0.0112764972	0.0130132512	-2.1514769694
H	0	0.010669859	0.0194306958	-3.2386222214

Nitrobenzene *ortho* anion 12

G3MP2 = -435.511110

C	0	-1.1968652441	-0.0625831801	-1.1834864071
C	0	-1.3295054405	-0.0867946474	0.2291773737
H	0	-2.1095073395	-0.1014551912	-1.7932655569
C	0	-0.058700527	-0.0125043679	0.806243371
N	0	0.0208552893	-0.0224234457	2.2953141017
O	0	0.9614511034	0.5960959569	2.845376613
O	0	-0.8333116615	-0.648137304	2.9446552952
C	0	1.1968605122	0.0729371964	0.1873519339
H	0	2.1134204417	0.1361437465	0.7693881146
C	0	1.2199176335	0.0697391031	-1.2044486006
H	0	2.1697727384	0.1161641371	-1.7367282617
C	0	0.0091452556	0.004055038	-1.8983405204
H	0	0.0115127796	0.0050528893	-2.9915031045

Nitrobenzene *meta* anion 13

G3MP2 = -435.504890

C	0	-1.4792184015	-0.1387322387	-1.2326115607
C	0	-0.1731128467	-0.0088033858	0.8934573199
N	0	-0.1673659746	-0.0095339215	2.351263995
O	0	0.923703134	0.099985452	2.95443268
O	0	-1.2503755055	-0.1193447465	2.962422502
C	0	1.0598091743	0.1161785998	0.2452128623
H	0	1.9776678828	0.2082868471	0.8165699652
C	0	1.0320176776	0.114582171	-1.1449379505
H	0	1.9732647253	0.2100004873	-1.6935060939
C	0	-0.1928482568	-0.0083856983	-1.8260938112
H	0	-0.1213049092	-0.0002052208	-2.9232330786
C	0	-1.3806642527	-0.1300384534	0.1855780073
H	0	-2.282551918	-0.2215922611	0.7955198955

Nitrobenzene *para* anion 14

G3MP2 = -435.506749

C	0	-0.1620823774	-0.0137255466	0.7126634308
N	0	-0.1843698629	-0.0237611426	2.160547771
O	0	0.8951363647	0.0722964582	2.7829658273
O	0	-1.2824996644	-0.1282047348	2.7480581068
C	0	1.0564001924	0.1021489295	0.0425442154
H	0	1.9776996147	0.1839010536	0.6151817749
C	0	1.0323285506	0.1075898545	-1.3574467239
H	0	2.0174965128	0.2009991197	-1.8336181285

C	0	-0.1173586653	0.0062860955	-2.1918199198
C	0	-1.3593239918	-0.1201773818	0.0038169317
H	0	-2.2977871417	-0.2097271613	0.5466402475
C	0	-1.2921683768	-0.1062320757	-1.3947127505
H	0	-2.2621751767	-0.1929560612	-1.9022402757

Benzonitrile

G3MP2 = -323.954023

C	0	-0.0053031116	-0.0026717966	0.6387279611
C	0	0.0993482589	-1.2278952474	-0.0341173718
H	0	0.1910601861	-2.1488774619	0.5351850672
C	0	0.0841741505	-1.2459991754	-1.4261819
H	0	0.1650873094	-2.1936790671	-1.9517688858
C	0	-0.1243988185	1.1962812804	-0.0776437072
H	0	-0.2046592281	2.138160611	0.458216391
C	0	-0.138114213	1.1617375201	-1.4694068733
H	0	-0.2303582944	2.0888913151	-2.0286586252
C	0	0.0095925894	0.0244450848	2.0725330226
N	0	0.0218662153	0.0467863124	3.2544832257
C	0	-0.0341903617	-0.0553125631	-2.1447569504
H	0	-0.0453929753	-0.0758535794	-3.2313512308

Benzonitrile *ortho* anion 15

G3MP2 = -323.346349

C	0	-0.2780265839	0.	0.9034510884
C	0	0.9558374963	0.	0.2172300202
H	0	1.9009377851	0.	0.7645004986
C	0	0.9446416745	0.	-1.173999705
H	0	1.8795846641	0.	-1.7346440028
C	0	-0.1829869671	0.	2.347997338
N	0	-0.0796379462	0.	3.5278547101
C	0	-0.2881202897	0.	-1.8314767379
H	0	-0.3154238715	0.	-2.9248974479
C	0	-1.4773863708	0.	-1.0863736439
C	0	-1.5819993833	0.	0.3303365018
H	0	-2.4053252706	0.	-1.6742784596

Benzonitrile *meta* anion 16

G3MP2 = -323.342407

C	0	-0.0034036851	0.	0.8011179099
C	0	1.2256005878	0.	0.1206015492
H	0	2.163835501	0.	0.6741207073

C	0	1.1906440544	0.	-1.2701132349
H	0	2.1310655151	0.	-1.8276666064
C	0	-0.00953035	0.	2.2321494148
N	0	-0.0290506531	0.	3.4176954371
C	0	-1.2193387215	0.	0.0744422257
H	0	-2.1287678279	0.	0.6895759798
C	0	-1.3335920146	0.	-1.3381538643
C	0	-0.0450548411	0.	-1.9407859143
H	0	0.018866009	0.	-3.0383108

Benzonitrile *para* anion 17

G3MP2 = -323.342845

C	0	-0.1778709813	0.	0.9539964323
C	0	1.0123423158	0.	0.2093425301
H	0	1.9702630291	0.	0.7345700545
C	0	0.9354026455	0.	-1.1885506321
H	0	1.9043650422	0.	-1.7064057478
C	0	-0.1412822062	0.	2.3826951677
N	0	-0.1109468724	0.	3.5669369026
C	0	-0.2527979308	0.	-1.9720281727
C	0	-1.4046365883	0.	0.2712335956
H	0	-2.3344215026	0.	0.8447974924
C	0	-1.3993427325	0.	-1.1287641738
H	0	-2.3935385064	0.	-1.5963508107

3-Methylpyridine N-oxide

G3MP2 = -362.187206

C	0	-0.0163293894	0.0026598718	1.1056698208
C	0	1.1674367334	-0.08999531	1.8165010748
C	0	-1.2268395825	0.0978770299	1.8031921555
C	0	-1.1927861801	0.0956562858	3.1956554944
H	0	-2.1692298378	0.1716530806	1.2675339307
H	0	2.1534847197	-0.1675137544	1.37263922
N	0	1.1981827714	-0.0919618199	3.1970182654
C	0	0.0036166183	0.0019960104	3.8792488864
H	0	-2.1084913812	0.1676990406	3.7757356473
O	0	2.2995701361	-0.1781859123	3.8190125126
H	0	0.1194616207	-0.0067455296	4.9558275887
C	0	0.0175882475	-0.0004790429	-0.3978203202
H	0	1.0406443539	-0.0807989794	-0.7723465164
H	0	-0.4195385194	0.9196621628	-0.7959665332
H	0	-0.5575997348	-0.8415226782	-0.7953964008

3-Methylpyrdine N-oxide benzylic anion 18

G3MP2 = -361.602243

C	0	-0.0619818413	-0.0763585077	-0.7864286337
C	0	-1.2187617367	0.0620694731	0.0556397674
C	0	1.1795407632	-0.1590642941	-0.0482416562
C	0	1.1874174883	-0.1043708954	1.3295243247
H	0	2.112987929	-0.2656526814	-0.600126788
H	0	-2.2275661225	0.1375527156	-0.3373967768
N	0	-1.1804255998	0.1130853681	1.4107317031
C	0	0.0192114388	0.0314430735	2.0795449535
H	0	2.1332608381	-0.1682783289	1.8689363483
O	0	-2.280764082	0.2402812201	2.0988523005
H	0	-0.0626087574	0.0821320874	3.1560039266
C	0	-0.1470798938	-0.1238060158	-2.1598026908
H	0	-1.101783652	-0.0580142627	-2.6728204679
H	0	0.7437899942	-0.2289562318	-2.7717493218

4-Methylpyrdine N-oxide

G3MP2 = -362.186332

C	0	0.5999640785	-0.0545220864	-1.0209081425
C	0	1.7653903876	-0.1993277657	-0.2953015326
C	0	-0.6444509991	0.0954445317	-0.4002780404
C	0	-0.6338319683	0.0824235803	0.9982873652
C	0	-1.9188500166	0.2111146856	-1.1867851809
H	0	2.7571488213	-0.3132878334	-0.7152918036
N	0	1.7519419066	-0.2087040854	1.0846433912
C	0	0.5348420469	-0.0627449583	1.7185640096
H	0	-1.5601849765	0.1951908621	1.5570078878
O	0	2.8226500764	-0.3418756422	1.7479274106
H	0	0.6098258973	-0.0749378259	2.7989311398
H	0	0.6779049791	-0.053219606	-2.1057748272
H	0	-1.7424588438	0.6966197786	-2.1504742631
H	0	-2.6627461759	0.8005624325	-0.6439167153
H	0	-2.3571452143	-0.7727360684	-1.3866306985

4-Methylpyrdine N-oxide benzylic anion 19

G3MP2 = -361.606476

C	0	0.6661238628	-0.0279178679	-1.0460741137
C	0	1.7986352392	-0.0882481036	-0.2663550873
C	0	-0.6689573963	-0.0330734218	-0.5004624784
C	0	-0.6419251908	-0.1083388731	0.9395945596
C	0	-1.8193666011	0.0262464152	-1.2558839815

H	0	2.8085113227	-0.0851482095	-0.6648230648
N	0	1.7609091064	-0.1583729707	1.0951246703
C	0	0.5237401495	-0.1666677815	1.6689824982
H	0	-1.5827092054	-0.1205997929	1.4894798389
O	0	2.8740470374	-0.215839028	1.8260709328
H	0	0.5572890997	-0.2234999189	2.752624943
H	0	0.7992033511	0.0259157932	-2.1263476798
H	0	-1.7802426376	0.0819881403	-2.3399522687
H	0	-2.8008597385	0.0191923243	-0.7906311486

N-Methoxypyridinium *ortho* zwitterion

G3MP2 = -362.110159

H	0	0.1626608245	-0.5060882755	-3.339862248
C	0	0.1284666937	-0.2765864478	-2.2773243023
C	0	-0.8991571415	0.4902782456	-1.7412631741
C	0	1.1286090997	-0.7541532217	-1.4230618168
H	0	-1.6741355774	0.8587839241	-2.4104016015
H	0	1.9561108335	-1.3574685625	-1.7813035037
C	0	-1.0173324372	0.8348172987	-0.3678881329
N	0	-0.0008111745	0.3145173003	0.3215837512
C	0	1.0523170263	-0.4434285906	-0.0836553657
H	0	1.7579736476	-0.7490669077	0.6795368851
O	0	0.0979228953	0.5256352437	1.7270663409
C	0	-0.9796077847	1.3194608527	2.2371439581
H	0	-0.9957681842	2.3118274278	1.7857329556
H	0	-0.7369729733	1.3706937192	3.2995212376
H	0	-1.9445755489	0.8390087845	2.0733794786

N-methoxypyridinium *ortho* zwitterion rotational transition state

G3MP2 = -362.095743

H	0	0.6158990443	-0.4084361881	-3.3359646002
C	0	0.3232815206	-0.2740889204	-2.2969028859
C	0	-1.0147005407	-0.1412060256	-1.9330559657
C	0	1.2888992048	-0.2311544645	-1.294277574
H	0	-1.7687569463	-0.1748553043	-2.7171280722
H	0	2.349262859	-0.3278217431	-1.5038299833
C	0	-1.4858187874	0.0368685603	-0.6085657046
N	0	-0.4505291175	0.0593804786	0.2520801202
C	0	0.8826421132	-0.0590536104	0.0168938928
H	0	1.5827995513	-0.017538119	0.8385160494
O	0	-0.9092293118	0.2381152425	1.5904777137

C	0	0.0913793267	0.2798416713	2.6042474011
H	0	0.6521402372	-0.6583162561	2.6773987756
H	0	-0.4951228663	0.420204658	3.5120598618
H	0	0.7761068568	1.1260388258	2.4815986653

Chlorobenzene

G3MP2 = -690.986074

C	0	-0.1838190942	0.	1.126253404
C	0	1.0181871631	0.	0.4216509633
H	0	1.9614538651	0.	0.9596741888
C	0	0.9866266832	0.	-0.9721892017
H	0	1.9215203902	0.	-1.5264387036
C	0	-0.2314559479	0.	-1.651737968
H	0	-0.2500823225	0.	-2.7380436519
C	0	-1.4255208169	0.	-0.9308289481
H	0	-2.3788678092	0.	-1.4526989053
Cl	0	-0.1539827214	0.	2.866192443
C	0	-1.4092736617	0.	0.4632780089
H	0	-2.3335400869	0.	1.0333239517

Chlorobenzene *ortho* anion

G3MP2 = -690.371199

C	-0.0281095609	0.	1.2575796595
C	1.2153345898	0.	0.6158860682
H	2.1524520078	0.	1.1715710293
C	1.2091253062	0.	-0.7801072066
H	2.1507467184	0.	-1.330122268
C	-0.0159158364	0.	-1.4489635452
H	-0.040081792	0.	-2.5418423063
C	-1.2051520776	0.	-0.7011573225
H	-2.1358081983	0.	-1.2860879455
Cl	0.1430959506	0.	3.0949012171
C	-1.2982953616	0.	0.7141704091

Deprotonated 2-pyridinol

G3MP2 = -322.469634

H	0.0142520192	-0.0269642486	0.0095037142
C	-0.0011797113	-0.000964294	1.102023797
C	1.1822900956	0.0064225607	1.8092536818
C	-1.2212787342	0.0250502377	1.7971972555
C	-1.1387126373	0.0572724725	3.1872704128
H	-2.182421096	0.0206462995	1.2877340029

H	2.1442445713	-0.0132101187	1.2989282434
C	1.212914154	0.0405043295	3.2597710986
N	-0.0173702788	0.0656855535	3.9186432724
H	-2.069428139	0.078359815	3.7689380959
O	2.2966600636	0.047197393	3.9017287977

2-Pyridinone

G3MP2 = -323.020751

H	-0.0048658842	-0.020382643	-2.2481058803
C	-0.0024374823	-0.0041773638	-1.1605802339
C	1.1901765805	0.0161280457	-0.4920426866
C	-1.2407029014	-0.0046002607	-0.4612800363
C	-1.2090147971	0.0159744731	0.9020913682
H	-2.1894657858	-0.0205752342	-0.9838813812
H	2.1393249949	0.0166060415	-1.0174723115
C	1.2585882603	0.0382805729	0.9545962394
H	-2.0963841453	0.0174631915	1.526779773
O	2.2777773009	0.0575778235	1.6511753348
N	-0.0104475668	0.0361097379	1.5555044349
H	0.0188288052	0.0515956155	2.5716475827

HCCCH=CH-C=N-O⁻

G3MP2 = -322.311553

H	-0.5760112552	-0.072331138	-0.0555791367
C	-0.4600403923	-0.0148555391	1.0012373736
C	-0.1428016699	0.0293764453	2.1875063207
C	0.0588648081	0.0978901878	3.5863361238
C	1.2619970348	0.0377426687	4.2508365146
H	-0.8420340335	0.2090655238	4.1889648029
C	2.6021939567	-0.1005282881	3.8134872544
H	1.1651408095	0.1119717425	5.3388120897
H	3.4090191002	-0.1225974397	4.5549165233
N	2.9423689595	-0.208026781	2.5170403628
O	4.2083546981	-0.3271889392	2.2930484849

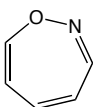
HCCCH=CH-C=N-OH

G3MP2 = -322.877162

H	-1.5635190134	-0.1270965162	-3.2276539434
C	-1.4672849708	-0.1070283083	-2.1654704566
C	-1.3414880853	-0.0832622367	-0.9493156248

C	-1.233277095	-0.0575359376	0.4690107826
C	-0.0572803824	0.0131561481	1.1365628884
H	-2.1605304345	-0.0977865193	1.0363686901
C	1.2322122163	0.0711082378	0.4871481525
H	-0.058828279	0.0284704274	2.223436284
H	1.3135105524	0.0599320133	-0.6007996012
N	2.2861567105	0.1366017532	1.2361336586
O	3.4399225197	0.1853483564	0.43564546
H	4.1478068415	0.2316239441	1.1028100557

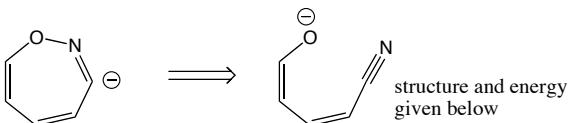
Seven-membered ring species (neutral)



G3MP2 = -322.904059

H	0.0508591934	-0.3991965859	-2.2303551087
C	0.1312939255	-0.2170099276	-1.1604048545
C	1.4074201467	0.1946191511	-0.6395079678
C	-0.9982982047	-0.3056150947	-0.402295832
H	2.1236136101	0.681837832	-1.2958459631
C	-1.0597625947	0.1762595102	0.9597786639
H	-1.9432245557	-0.5395901655	-0.8860400428
N	-0.1510567278	0.1362294685	1.885259585
H	-1.9389786515	0.7451057618	1.2664678319
O	0.9278635905	-0.7707570301	1.4609850387
C	1.7479338568	-0.0132866723	0.6525329384
H	2.6876094795	0.3093763846	1.0971610901

Seven-membered ring species (anion 1)

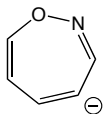


G3MP2 = -322.4334

H	0.4211964285	0.058161064	-2.07163674
C	0.2732543623	0.0403708852	-0.9860084739
C	-1.080542241	-0.0610521602	-0.6217487139
C	1.4802280592	0.1244217942	-0.3171232852
H	-1.8028179444	-0.1087278213	-1.4357074216
C	1.7770319638	0.1371887138	1.0675390876
H	2.3724579124	0.1937135226	-0.937030546
N	2.2309790516	0.1632868447	2.16565766
O	-1.016181416	-0.0715324555	1.7794301208

C	-1.6172166511	-0.1085937128	0.6830838877
H	-2.7379493343	-0.1906958229	0.6943835545

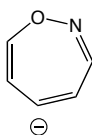
Seven-membered ring species (anion 2)



G3MP2 = -322.297226

H	0.3911504737	-0.4221237849	-2.3944050519
C	0.3706496254	-0.1750183995	-1.3226998501
C	-0.9287566422	0.1833488466	-0.7769667631
C	1.5263174554	-0.2102726413	-0.5835565093
H	-1.6584385033	0.770332625	-1.3459850896
C	1.4173804398	0.1808056832	0.7845155169
N	0.6168167352	-0.1479757554	1.7795449518
H	2.1834460422	0.8711662849	1.1707177578
O	-0.4716601032	-1.0300248836	1.2183289538
C	-1.2641840959	-0.1770185406	0.4881770941
H	-2.1827214281	0.1567804586	0.9823289895

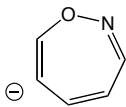
Seven-membered ring species (anion 3)



G3MP2 = -322.292145

C	0.1412595261	0.3396102338	-1.5171049209
C	-1.0674404052	-0.1539745273	-0.8893889993
C	1.2300917124	0.4031180547	-0.6694556193
H	-1.7966761314	-0.6907148394	-1.5092927983
C	1.3023771339	-0.1736642928	0.6565457465
H	2.2057775668	0.7153164434	-1.0679437778
N	0.4052176352	-0.2034275248	1.606822528
H	2.1628353332	-0.8079411616	0.9170279223
O	-0.6649538979	0.7566079386	1.280556143
C	-1.4700647987	0.048875175	0.3958002684
H	-2.4484236744	-0.2338055006	0.7964335073

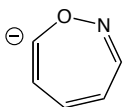
Seven-membered ring species (anion 4)



G3MP2 = -322.302549

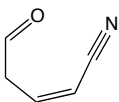
H	0.1639689394	0.4738772918	-2.2883510446
C	0.0711633493	0.1916732198	-1.2312117441
C	-1.1413868313	-0.2984019267	-0.7393781394
C	1.2533796777	0.1459514604	-0.4790763924
C	1.2826170943	-0.0837503529	0.9167244196
H	2.2198342922	0.119401056	-0.9915026537
N	0.3658972596	0.0930807274	1.8660149262
H	2.187302411	-0.5282383351	1.3476648672
O	-0.7715838902	0.8274692426	1.3754207146
C	-1.4600136943	-0.1639196813	0.5482524926
H	-2.1762638688	-0.7403663811	1.1350607311

Seven-membered ring species (anion 5)



G3MP2 = -322.288691

H	0.112276793	-0.3918259994	-2.1638081367
C	0.1494290631	-0.2119393517	-1.0833049621
C	1.37442165	0.2614089191	-0.5248350187
C	-1.0317411922	-0.3415338635	-0.3914452919
H	2.0746916673	0.707902299	-1.238543402
C	1.8313074151	0.2072940832	0.7882978101
C	-1.1486931946	0.1513932432	0.9455121607
H	-1.9480776692	-0.5827696862	-0.931497342
N	-0.2058498756	0.2088361425	1.8559512235
H	-2.0653684598	0.6753559856	1.2364777043
O	0.857603751	-0.6841217707	1.5071952548



G3MP2 = -322.971882

C	1.3752248666	0.0603849345	-2.4979697131
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N	2.3187539815	0.1419540911	-3.2063294085
C	0.2261860993	-0.0337696386	-1.6517124778
C	0.3159650398	-0.0590458427	-0.3096928688
H	-0.7404986175	-0.0737122273	-2.1448823227
C	1.591519865	-0.0169296293	0.4698851741
H	-0.6122131828	-0.1256661723	0.2556866405
H	2.4710776746	0.0215866838	-0.1778569915
C	1.7127218311	-1.2241122472	1.3772490928
H	1.5953833239	0.876909892	1.1118413071
O	2.7134906135	-1.9174218992	1.4556756807
H	0.8166525792	-1.4462714347	1.9927744192