1. CH3NO2 MP2/6-311+G**

	X	Y	Z
C	-1.303451	-.000038	-.027344
N	.051351	.000006	.001171
O	.690564	1.106289	.001645
O	.690635	-1.106252	.001645
H	-1.794205	.956487	.064776
H	-1.794141	-.956593	.064777

2. CH2NO2 anion MP2/6-311+G**

	X	Y	Z
C	-1.303451	-.000038	-.027344
N	.051351	.000006	.001171
O	.690564	1.106289	.001645
O	.690635	-1.106252	.001645
H	-1.794205	.956487	.064776
H	-1.794141	-.956593	.064777

3. Ch3CH2NO2 MP2/6-311+G**

	X	Y	Z
C	.690643	-.507666	.517072
N	-.636983	.021070	.061885
O	-.780631	1.243200	.081707
O	-1.485000	-.792490	-.308180
H	.788784	-.203114	1.561148
C	1.799295	.074850	-.344174
H	.621854	-1.592219	.444455
H	1.824946	1.161256	-.251609
H	1.648871	-.189847	-1.393790

4. CH3CHNO2 anion MP2/6-311+G**

	X	Y	Z
C	-1.303451	-.000038	-.027344
N	.051351	.000006	.001171
O	.690564	1.106289	.001645
O	.690635	-1.106252	.001645
H	-1.794205	.956487	.064776
H	-1.794141	-.956593	.064777

5. CH3NO2 + OH- complex2 MP2/6-311+G**

	X	Y	Z
C	-2.009100	-0.000518	0.302022
N	-0.719067	0.000069	-0.077338
O	-0.097291	-1.109455	-0.255522
O	-0.098129	1.110041	-0.255241
H	-2.490611	-0.959648	0.406070
H	-2.491419	0.958187	0.406255
H	1.851339	-0.717382	0.088911
O	2.491089	-0.000243	0.228076
H	1.853415	0.718729	0.089494

6. CH3CH2NO2 + OH- complex2 MP2/6-311+G**

	X	Y	Z
C	-1.508891	.588599	.000568
N	-.201297	.279738	-.000826
O	.153736	-.955912	-.002099
O	.693363	1.209622	-.000925
C	-2.514223	-.511711	.001107
H	-1.740089	1.644226	.002039
H	-2.408594	-1.165215	.878547
H	-2.409845	-1.164762	-.876798
H	-3.525342	-.087474	.001947

H	2.318139	-1.046577	.000405
O	3.015805	-.377244	.001595
H	2.410254	.388584	.001035

7. CH3NO2 + CN- complex1 MP2/6-311+G**

	X	Y	Z
C	-.073196	-.002341	-.059249
N	1.419635	.000121	-.010472
O	2.000437	-1.088546	.026474
O	1.996033	1.090945	.030253
H	-.448434	.005548	.963602
H	-.402258	-.906110	-.560989
H	-.404919	.892711	-.574812
C	-3.149365	-.004736	.652500
N	-3.045461	.004325	-.538259

8. CH3NO2 + CN- TS MP2/6-311+G**

	X	Y	Z
C	.356311	-.000013	1.097338
N	1.265460	.000001	.018629
O	1.611561	1.094390	-.484658
O	1.611566	-1.094377	-.484681
H	-.994431	-.000010	.464276
H	.441415	.923480	1.665877
H	.441420	-.923516	1.665858
C	-2.208507	-.000006	-.035483
N	-3.345495	.000007	-.363262

9. CH3NO2 + CN- complex2 MP2/6-311+G**

	X	Y	Z
C	-2.448434	-.389404	.349459
N	-1.245007	.042519	-.061004
O	-.336958	-.828879	-.380082
O	-.967623	1.279163	-.140219
H	1.238175	-.278410	-.121758
H	-2.605816	-1.455091	.382921
H	-3.185812	.362631	.581535
C	2.333369	-.100887	.037189
N	3.485076	.058958	.203836

10. CH3CH2NO2 + CN- complex1 MP2/6-311+G**

	X	Y	Z
C	.040544	-.075750	-.200856
N	1.504781	-.235574	.071942
O	1.975345	.371732	1.036951
O	2.170058	-.953068	-.683671
C	-.282170	1.385296	-.458190
H	-.506891	-.445967	.667778
H	-.179741	-.708393	-1.058079
C	-3.385670	-.201918	-.337421
N	-2.875015	-.626779	.656551
H	.274562	1.762937	-1.322437
H	-.040652	1.989485	.418715
H	-1.355092	1.443325	-.652865

11. CH3CH2NO2 + CN- TS MP2/6-311+G**

	X	Y	Z
C	.334517	.476928	-.673305
N	1.212978	-.381688	.008348
O	1.632818	-1.415504	-.568107
O	1.472025	-.142852	1.214255
H	-.990991	-.048830	-.333500

H	.473628	.364988	-1.746796
C	.251771	1.875029	-.116533
C	-2.224267	-.354773	.015808
N	-3.375770	-.553698	.203001
H	1.233668	2.355464	-.004414
H	-.361365	2.486575	-.788771
H	-.226259	1.873254	.869025

12. CH3CH2NO2 + CN- complex2 MP2/6-311+G**

	X	Y	Z
C	2.027968	.282574	-.214088
N	.743075	.518150	.094841
O	.010982	-.486686	.480606
O	.224465	1.679051	.023446
H	-1.633833	-.269529	.151303
C	2.560066	-1.108314	-.140879
H	2.592482	1.147735	-.532925
C	-2.737509	-.316326	-.035876
N	-3.893473	-.393704	-.229429
H	2.018885	-1.793595	-.807849
H	2.469323	-1.531098	.868747
H	3.619208	-1.111152	-.424504

13. C6H5CH2NO2 B3LYP/6-31+G*

	X	Y	Z
C	1.195901	-0.000430	1.026668
N	2.175098	-0.000005	-0.143048
O	2.526758	-1.091931	-0.581119
O	2.526686	1.092250	-0.580372
H	1.432068	-0.899141	1.596950
C	-0.226172	-0.000190	0.522799
H	1.432140	0.897821	1.597648
C	-0.890278	1.210444	0.282238
C	-2.202329	1.210269	-0.195291
C	-2.860279	0.000240	-0.434393
C	-2.202700	-1.210006	-0.195356
C	-0.890650	-1.210610	0.282165
H	-0.377288	2.151748	0.463246
H	-2.709989	2.153468	-0.378541
H	-3.882538	0.000402	-0.803471
H	-2.710658	-2.153034	-0.378661
H	-0.377944	-2.152079	0.463120

14. C6H5CHNO2 anion B3LYP/6-31+G*

	X	Y	Z
C	-1.149218	-0.758872	0.000004
N	-2.269219	0.011846	0.000074
O	-2.199120	1.286529	-0.000078
O	-3.410263	-0.568949	0.000012
C	0.214564	-0.322725	-0.000012
H	-1.369315	-1.818637	0.000020
C	1.226850	-1.328939	-0.000028
C	2.582014	-1.018108	-0.000014
C	3.011057	0.318383	0.000012
C	2.034743	1.323914	0.000025
C	0.672060	1.026926	0.000012
H	0.919197	-2.374143	-0.000045
H	3.314217	-1.825610	-0.000024
H	4.070982	0.565196	0.000017
H	2.341033	2.370180	0.000042
H	-0.068941	1.815971	0.000005

15. p-CH3OC6H4CH2NO2 B3LYP/6-31+G*

	X	Y	Z
C	-2.168292	0.017075	0.972248
N	-3.001189	-0.162448	-0.295836
O	-3.397943	0.855148	-0.857493
O	-3.197020	-1.311894	-0.681939
C	-0.704002	0.108901	0.636429
H	-2.398781	-0.853189	1.587573
C	0.090773	-1.040072	0.586008
C	1.448197	-0.968812	0.260397
C	2.026144	0.276592	-0.021875
C	1.237136	1.438022	0.027033
C	-0.110091	1.350606	0.351925
H	-0.350852	-2.010908	0.797246
H	2.035372	-1.879611	0.232769
O	3.335937	0.464674	-0.347088
H	1.702336	2.394197	-0.192140
H	-0.712179	2.255395	0.380103
C	4.191683	-0.669821	-0.429797
H	5.171700	-0.279733	-0.708599
H	4.264567	-1.184360	0.537020
H	3.845714	-1.373416	-1.197741
H	-2.546621	0.930386	1.432557

16. p-CH3OC6H4CHNO2 anion B3LYP/6-31+G*

	X	Y	Z
C	2.074746	-0.770763	0.000054
N	3.180779	0.013065	0.000106
O	3.091650	1.289756	-0.000041
O	4.333330	-0.549453	-0.000062
C	0.701902	-0.349232	0.000020
H	2.305380	-1.828446	0.000027
C	-0.302757	-1.352526	-0.000027
C	-1.668897	-1.059541	-0.000060
C	-2.093696	0.274028	-0.000043
C	-1.129870	1.289359	0.000005
C	0.230641	0.996130	0.000034
H	0.002789	-2.398036	-0.000038
H	-2.381600	-1.879600	-0.000098
O	-3.425313	0.682385	-0.000090
H	-1.466062	2.324416	0.000019
H	0.965331	1.791217	0.000075
C	-4.414204	-0.320832	0.000086
H	-5.377284	0.198229	0.000136
H	-4.349354	-0.960308	-0.894181
H	-4.349172	-0.960164	0.894442

17. p-NO2C6H4CH2NO2 B3LYP/6-31+G*

	X	Y	Z
C	-2.427798	-0.006439	0.966083
N	-3.238310	0.002206	-0.326521
O	-3.518871	1.098024	-0.801687
O	-3.530141	-1.087103	-0.809654
C	-0.952259	-0.004143	0.650654
H	-2.734237	-0.908194	1.496005
C	-0.262148	-1.215373	0.497128
C	1.098991	-1.221898	0.198739
C	1.756369	-0.000477	0.057715
C	1.096435	1.219148	0.202756
C	-0.264638	1.209004	0.501156
H	-0.790985	-2.157896	0.606786
H	1.647802	-2.148102	0.078290

N	3.200754	0.001519	-0.250189
H	1.643399	2.146842	0.085373
H	-0.795275	2.150127	0.613961
O	3.760416	-1.088210	-0.370997
O	3.758219	1.092780	-0.367238
H	-2.734508	0.888287	1.507782

18. p-NO2C6H4CHNO2 anion B3LYP/6-31+G*

	X	Y	Z
C	2.342187	0.730509	0.000311
N	3.409180	-0.142855	0.000597
O	3.231861	-1.394447	-0.000467
O	4.575936	0.353645	-0.000168
C	0.968085	0.411917	0.000035
H	2.659678	1.764721	0.000289
C	0.042233	1.511295	-0.000113
C	-1.321765	1.328417	-0.000193
C	-1.853394	0.020415	-0.000152
C	-0.976813	-1.084026	-0.000002
C	0.392070	-0.901722	0.000075
H	0.441233	2.523723	-0.000160
H	-2.000191	2.174238	-0.000320
N	-3.262696	-0.177167	-0.000264
H	-1.396722	-2.084019	0.000024
H	1.058452	-1.753655	0.000136
O	-4.013846	0.825033	0.000115
O	-3.711883	-1.344942	0.000261

19. C6H5CH2NO2 + CN- complex1 B3LYP/6-31+G*

	X	Y	Z
C	0.851072	-0.591307	-0.636763
N	1.259359	-1.744474	0.245292
O	0.926965	-1.729297	1.429427
O	1.951332	-2.630720	-0.268526
H	1.608002	0.210727	-0.464838
C	-0.538813	-0.092681	-0.334570
H	0.959557	-0.970136	-1.654315
C	2.662739	2.074681	-0.250402
N	3.131706	3.154328	-0.168947
C	-1.668262	-0.839843	-0.701403
C	-2.953667	-0.366343	-0.430692
C	-3.121687	0.869981	0.203279
C	-2.000277	1.624594	0.559113
C	-0.712986	1.147428	0.293320
H	-1.539012	-1.800407	-1.198048
H	-3.821560	-0.957376	-0.716143
H	-4.122231	1.243593	0.412371
H	-2.123914	2.591026	1.042542
H	0.166614	1.734685	0.545516

20. C6H5CH2NO2 + CN- TS B3LYP/6-31+G*

	X	Y	Z
C	-0.875219	-0.249088	0.640114
N	-1.684599	-1.296239	0.083793
O	-1.460582	-1.715797	-1.069571
O	-2.660718	-1.689122	0.757338
H	-1.464024	0.876778	0.203775
C	0.564001	-0.161814	0.288113
H	-1.065099	-0.227427	1.712215
C	-2.054307	2.157554	-0.194523
N	-2.508077	3.212802	-0.428409
C	1.468746	0.195764	1.309196

C	2.827360	0.384093	1.050506
C	3.326470	0.216502	-0.244877
C	2.440573	-0.128516	-1.270735
C	1.078783	-0.306218	-1.016475
H	1.094705	0.325513	2.323101
H	3.496689	0.657345	1.864386
H	4.385138	0.358643	-0.452251
H	2.810010	-0.251020	-2.287377
H	0.403271	-0.566075	-1.821577

21. C6H5CH2NO2 + CN- complex2 B3LYP/6-31+G*

	X	Y	Z
C	-0.004871	-0.969564	-0.000080
N	1.186761	-0.344545	-0.000302
O	1.301597	0.924769	-0.000457
O	2.260984	-1.076384	-0.000400
H	3.790698	-0.164766	0.000002
C	-1.307978	-0.361052	0.000004
H	0.080479	-2.048204	0.000028
C	4.841110	0.200889	0.000273
N	5.944452	0.562797	0.000537
C	-2.433534	-1.231671	0.000181
C	-3.738316	-0.749430	0.000268
C	-3.988150	0.630496	0.000182
C	-2.894475	1.504815	0.000010
C	-1.581178	1.033582	-0.000078
H	-2.261071	-2.307074	0.000246
H	-4.568882	-1.454355	0.000401
H	-5.007467	1.011182	0.000247
H	-3.064908	2.580869	-0.000055
H	-0.743631	1.719108	-0.000204

22. p-CH3OC6H4CH2NO2 + CN- complex1 B3LYP/6-31+G*

	X	Y	Z
C	1.870170	-0.361326	-0.608514
N	2.576076	-1.271268	0.371265
O	2.158136	-1.337626	1.525701
O	3.573945	-1.874444	-0.039545
H	2.294751	0.654577	-0.439074
C	0.376488	-0.352353	-0.429218
H	2.187870	-0.720209	-1.589026
C	2.566094	2.814815	-0.248108
N	2.464574	3.987026	-0.155957
C	-0.411719	-1.458904	-0.787781
C	-1.794042	-1.437942	-0.633764
C	-2.419443	-0.291544	-0.120661
C	-1.651462	0.823371	0.229284
C	-0.260187	0.784647	0.074619
H	0.063636	-2.352750	-1.188920
H	-2.407062	-2.292748	-0.906212
O	-3.789803	-0.360475	-0.006530
H	-2.110663	1.726523	0.616416
H	0.340241	1.656284	0.324817
C	-4.473250	0.769432	0.509612
H	-5.531969	0.499470	0.519191
H	-4.147357	1.004291	1.532159
H	-4.328115	1.653422	-0.126347

23. p-CH3OC6H4CH2NO2 + CN- TS B3LYP/6-31+G*

	X	Y	Z
C	-1.728737	-0.228849	0.651178
N	-2.604320	-1.208144	0.081968

O	-2.397064	-1.637957	-1.072474
O	-3.618037	-1.531386	0.739522
H	-2.243435	0.956585	0.224756
C	-0.287579	-0.237892	0.294540
H	-1.916446	-0.203631	1.723658
C	-2.721282	2.266436	-0.148618
N	-3.088223	3.358562	-0.362820
C	0.655401	-0.022067	1.311946
C	2.028916	0.076039	1.054123
C	2.490991	-0.048132	-0.258581
C	1.569914	-0.255985	-1.292964
C	0.207024	-0.338343	-1.024489
H	0.312188	0.072230	2.340479
H	2.711552	0.241314	1.881535
O	3.820338	0.021830	-0.632270
H	1.939859	-0.338442	-2.311785
H	-0.491698	-0.492158	-1.837276
C	4.778400	0.270017	0.376869
H	5.747443	0.302825	-0.127831
H	4.597962	1.231622	0.879006
H	4.790196	-0.530505	1.131170

24. p-CH3OC6H4CH2NO2 + CN- complex2 B3LYP/6-31+G*

	X	Y	Z
C	-0.988269	1.047891	-0.000277
N	-2.146639	0.369907	-0.000155
O	-2.201835	-0.906008	0.000325
O	-3.257156	1.049917	-0.000728
H	-4.732696	0.069609	0.000028
C	0.343701	0.496331	-0.000217
H	-1.120116	2.121957	-0.000632
C	-5.765588	-0.347019	0.000428
N	-6.850408	-0.761523	0.000861
C	1.432013	1.401990	0.000078
C	2.764304	0.981412	0.000006
C	3.058546	-0.386889	-0.000325
C	2.004109	-1.307941	-0.000623
C	0.678151	-0.885927	-0.000590
H	1.225229	2.471056	0.000358
H	3.552158	1.728755	0.000215
O	4.340481	-0.918448	-0.000558
H	2.241786	-2.369402	-0.000898
H	-0.129049	-1.607214	-0.000855
C	5.425386	-0.016132	0.001350
H	6.331015	-0.628981	0.001775
H	5.423451	0.625532	-0.892837
H	5.421512	0.624012	0.896614

25. p-NO2C6H4CH2NO2 + CN- complex1 B3LYP/6-31+G*

	X	Y	Z
C	2.089376	-0.384992	-0.594867
N	2.721201	-1.414246	0.297464
O	2.279950	-1.554803	1.438423
O	3.689302	-2.032869	-0.154776
H	2.601523	0.586370	-0.375818
C	0.600624	-0.265600	-0.382561
H	2.348258	-0.689555	-1.610919
C	3.034734	2.624732	-0.168457
N	2.983156	3.800117	-0.087027
C	-0.254220	-1.353481	-0.629119
C	-1.629665	-1.233632	-0.465531
C	-2.147665	-0.000366	-0.057321

C	-1.323750	1.099419	0.187085
C	0.055017	0.960416	0.023676
H	0.162591	-2.307149	-0.945044
H	-2.298163	-2.066326	-0.648190
N	-3.598686	0.135503	0.112770
H	-1.756466	2.042584	0.499098
H	0.721447	1.802967	0.195949
O	-4.307504	-0.851524	-0.117846
O	-4.044948	1.227011	0.477328

26. p-NO2C6H4CH2NO2 + CN- TS B3LYP/6-31+G*

	X	Y	Z
C	-1.988963	-0.200297	0.638354
N	-2.798157	-1.260251	0.046251
O	-2.533318	-1.674560	-1.092689
O	-3.782486	-1.646061	0.696054
H	-2.474077	0.863095	0.172300
C	-0.529620	-0.198329	0.381809
H	-2.237778	-0.176258	1.698347
C	-3.044529	2.259538	-0.330922
N	-3.441552	3.324939	-0.623441
C	0.322626	0.147323	1.454250
C	1.697675	0.249488	1.292356
C	2.248450	0.002564	0.030304
C	1.433055	-0.322596	-1.059361
C	0.057044	-0.411575	-0.884960
H	-0.108939	0.333632	2.434343
H	2.345409	0.506293	2.122148
N	3.689828	0.088513	-0.149582
H	1.881945	-0.491061	-2.031194
H	-0.578366	-0.653567	-1.726420
O	4.388734	0.381018	0.831447
O	4.157889	-0.136803	-1.273950

27. p-NO2C6H4CH2NO2 + CN- complex2 B3LYP/6-31+G*

	X	Y	Z
C	-1.260297	1.114167	-0.000009
N	-2.405109	0.373876	-0.000045
O	-2.396571	-0.890186	0.000035
O	-3.522101	1.009169	-0.000125
H	-5.043425	-0.059724	-0.000088
C	0.073392	0.631616	0.000037
H	-1.452926	2.178282	-0.000040
C	-6.049291	-0.507191	-0.000016
N	-7.116088	-0.963233	0.000026
C	1.118490	1.611191	0.000031
C	2.452806	1.265042	0.000063
C	2.816372	-0.095840	0.000042
C	1.818762	-1.087383	0.000131
C	0.479954	-0.739136	0.000117
H	0.844165	2.663844	-0.000047
H	3.228485	2.022159	0.000012
N	4.199972	-0.464997	0.000012
H	2.115014	-2.130321	0.000126
H	-0.284535	-1.504012	0.000138
O	5.061457	0.438515	-0.000006
O	4.499799	-1.675565	-0.000206