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jo010042L
OCT 05 2001
Journal of Organic Chemistry

Table 1. Minimum energy conformations of NdMO obtained at the MP2/6-31G* level.

ttt
MP2=-415.9748996

C	.000000	.000000	.000000
N	.000000	.000000	1.448014
C	1.130176	.000000	2.179468
C	.829442	-.000377	3.682764
N	1.959617	-.001758	4.414217
C	1.959618	-.002973	5.862231
H	1.040585	-.003460	-.324757
H	-.503825	-.889327	-.388145
H	-.497817	.892673	-.388295
H	-.862123	-.000496	1.984643
O	2.291175	.000012	1.745149
O	-.331557	-.000206	4.117084
H	2.821739	-.002418	3.877587
H	.919030	-.005877	6.186985
H	2.462746	-.893014	6.249646
H	2.458135	.888991	6.251257

ctt
MP2=-415.9644094

C	.000000	.000000	.000000
N	.000000	.000000	1.460996
C	1.030036	.000000	2.337984
C	2.452434	.002585	1.764108
N	3.362985	.002117	2.760454
C	4.789195	.004822	2.514380
H	.498206	.883712	-.397094
H	.499394	-.883002	-.397293
H	-1.044903	-.000696	-.314981
H	-.897172	-.002464	1.934150
O	.856497	-.001727	3.567915
O	2.706586	.004704	.552210
H	2.978739	.000782	3.700156
H	4.933143	.004921	1.433886
H	5.255819	.896514	2.942051
H	5.259054	-.884982	2.942394

csc
MP2=-415.9536118

C	.000000	.000000	.000000
N	.000000	.000000	1.457936
C	1.048338	.000000	2.318957
C	2.437338	.042724	1.687477
N	3.379752	.747073	2.362902
C	3.274730	1.448202	3.636901
H	.758092	.681138	-.381584
H	.196098	-.993965	-.407163
H	-.982716	.344955	-.327257
H	-.887034	-.130397	1.933136
O	.905745	-.071584	3.547384
O	2.682752	-.569836	.639134
H	4.300363	.653751	1.946469
H	2.333979	1.991975	3.696871
H	3.328886	.762390	4.484770
H	4.099616	2.161575	3.686646

Table 2. Atomic coordinates for the most relevant structures of the rotational profiles computed for NdMO at the MP2/6-31G(d) level.

ω1= 90°
MP2=-415.9448488

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.480084
C	1.297202	0.000000	2.007804
C	1.903116	1.396054	2.254298
N	3.178127	1.338773	2.685043
C	3.979512	2.523147	2.922041
H	0.491747	0.887461	-0.415591
H	0.507692	-0.899260	-0.352602
H	-1.035942	-0.030154	-0.340212
H	-0.409032	0.896716	1.756819
O	1.995686	-1.005422	2.111524
O	1.246576	2.422351	2.031079
H	3.569330	0.407975	2.783815
H	3.327065	3.387587	2.800316
H	4.385075	2.512544	3.936665
H	4.803548	2.589136	2.206055

ω1= 0°
MP2=-415.9644093

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.460997
C	1.030046	0.000000	2.337960
C	2.452423	0.000000	1.763997
N	3.363063	0.000015	2.760255
C	4.789251	0.001089	2.514017
H	0.498197	0.883670	-0.397302
H	0.499450	-0.883029	-0.397064
H	-1.044900	-0.000834	-0.314986
H	-0.897174	0.001355	1.934152
O	0.856508	0.000263	3.567893
O	2.706508	0.000134	0.552084
H	2.978898	0.000401	3.699989
H	5.257145	0.890875	2.944209
H	5.257943	-0.890615	2.939400
H	4.933093	0.003968	1.433512

ω2= 90°
MP2=-415.9541815

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.454536
C	1.174052	0.000000	2.145728
C	1.001538	0.176612	3.652144
N	0.859458	-0.996543	4.330338
C	0.845686	-1.009316	5.784859
H	0.817896	-0.636231	-0.336372
H	-0.948489	-0.403257	-0.358059
H	0.147962	1.004406	-0.409827
H	-0.818911	0.352471	1.936131
O	2.283748	-0.181833	1.638999
O	0.941986	1.294512	4.169777
H	1.124929	-1.845056	3.844129
H	0.290788	-0.135433	6.124476
H	0.346692	-1.916252	6.129581
H	1.855864	-0.965811	6.204781

ω2= 0°

MP2=-415.9450245

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.453785
C	1.170101	0.000000	2.164269
C	1.099821	-0.000361	3.711237
N	-0.130254	-0.000668	4.312547
C	-0.262215	-0.000871	5.760306
H	1.040782	-0.003859	-0.319814
H	-0.502059	-0.890217	-0.388834
H	-0.495359	0.893827	-0.389220
H	-0.896577	0.000009	1.912984
O	2.275741	0.000141	1.629299
O	2.152345	-0.000324	4.344317
H	-0.981639	-0.000786	3.774137
H	0.745177	0.003526	6.173390
H	-0.798009	0.888998	6.102116
H	-0.790357	-0.895013	6.102968