

XYZ coordinates in Ångstrom of the ground state optimized structures of NATMA A, NATMA B and NATMA C.

NATMA A:

36

FINAL HEAT OF FORMATION = -855.966444

C	1.931665	-0.687825	1.273429
C	1.655953	0.477912	0.516005
C	2.730841	1.142936	-0.156477
C	4.059109	0.674615	-0.099254
C	4.302211	-0.476851	0.657560
C	3.249616	-1.149579	1.335955
C	0.451246	1.222973	0.246427
C	0.828844	2.286915	-0.569040
N	2.189014	2.229497	-0.813433
C	-0.938263	0.872053	0.686286
C	-1.656254	-0.082903	-0.304530
N	-2.969709	-0.456427	0.171215
C	-0.854750	-1.374282	-0.468640
O	-1.037472	-2.331825	0.289604
N	0.045112	-1.360139	-1.490722
H	2.716576	2.923220	-1.330707
H	0.219536	3.092259	-0.983082
H	4.872736	1.192033	-0.619787
H	5.323363	-0.866186	0.728001
H	3.479102	-2.049420	1.916573
H	1.123626	-1.229256	1.777602
H	-0.915197	0.376165	1.673270
H	-1.566112	1.774300	0.772012

H	-1.766968	0.444015	-1.268654
H	-3.028001	-1.349098	0.654958
H	0.223419	-0.453422	-1.912693
C	1.068120	-2.385757	-1.622261
H	2.038015	-2.033933	-1.230550
H	0.739970	-3.253478	-1.033709
H	1.178773	-2.681513	-2.677565
C	-4.014998	0.423038	0.120686
O	-3.909479	1.540036	-0.388362
C	-5.305481	-0.078852	0.747244
H	-5.421449	0.380970	1.742542
H	-6.149706	0.251847	0.125109
H	-5.330458	-1.173923	0.855739

NATMA B:

36

FINAL HEAT OF FORMATION = -855.966719

C	-1.369508	-1.820593	-0.382091
C	-1.615787	-0.625672	0.342713
C	-2.941554	-0.086948	0.385440
C	-4.021906	-0.700663	-0.280267
C	-3.751423	-1.873330	-0.993432
C	-2.442395	-2.426178	-1.041891
C	-0.774038	0.239391	1.132361
C	-1.599127	1.250543	1.614705
N	-2.891379	1.054690	1.161049
C	0.704741	0.076974	1.306778
C	1.468517	0.240451	-0.035182

N	2.843060	-0.185550	0.084978
C	1.474009	1.702544	-0.480577
O	2.455120	2.428943	-0.298994
N	0.316315	2.108220	-1.073967
H	-3.689652	1.625638	1.413689
H	-1.353711	2.101288	2.252412
H	-5.034076	-0.283032	-0.239761
H	-4.567270	-2.377509	-1.522131
H	-2.275870	-3.350434	-1.605061
H	-0.363416	-2.256954	-0.408333
H	1.107707	0.803229	2.035371
H	0.931655	-0.938501	1.674472
H	0.968124	-0.386519	-0.793350
H	3.541612	0.553762	0.099803
H	-0.467983	1.462266	-1.036423
C	0.058018	3.505778	-1.370985
H	-0.398467	3.609351	-2.367777
H	-0.609722	3.965883	-0.620961
H	1.022886	4.030809	-1.356109
C	3.162493	-1.511001	0.019809
O	2.303119	-2.391428	-0.075723
C	4.649378	-1.819946	0.054865
H	4.813529	-2.689270	0.708271
H	4.979062	-2.097010	-0.959768
H	5.254292	-0.970993	0.408087

NATMA C:

FINAL HEAT OF FORMATION = -855.969025

C	-2.367474	1.069833	0.893180
C	-1.951584	-0.215519	0.456795
C	-2.755028	-0.911689	-0.505752
C	-3.943419	-0.366425	-1.031741
C	-4.324780	0.902074	-0.582788
C	-3.544492	1.612552	0.369571
C	-0.821289	-1.057873	0.764120
C	-0.970459	-2.204473	-0.010574
N	-2.129341	-2.112871	-0.756450
C	0.306711	-0.727549	1.703249
C	1.479120	-0.026820	0.996795
N	0.963533	1.052200	0.160952
C	2.331724	-1.038979	0.198702
O	2.053894	-2.240209	0.139768
N	3.414262	-0.465752	-0.392128
H	-2.458679	-2.820110	-1.403494
H	-0.307729	-3.065167	-0.087591
H	-4.547039	-0.911706	-1.765821
H	-5.242141	1.355818	-0.972068
H	-3.877099	2.602347	0.699999
H	-1.775589	1.627322	1.628271
H	-0.067705	-0.063127	2.501239
H	0.693731	-1.642299	2.177314
H	2.148499	0.444010	1.740795
H	0.029498	0.930006	-0.224905
H	3.561062	0.532651	-0.225958
C	4.352230	-1.229478	-1.191918
H	4.431357	-0.817799	-2.212045

H	5.356465	-1.235546	-0.735226
H	3.979299	-2.261687	-1.245699
C	1.685185	2.161655	-0.155297
O	2.868113	2.309036	0.181579
C	0.938156	3.206601	-0.963861
H	1.162372	4.197093	-0.540718
H	1.315786	3.194411	-1.999349
H	-0.150549	3.044119	-0.971960