Supplementary Material

Experimental and density functional theory studies of the novel piperidine-containing acetylene glycols

Amina Mirsakiyeva,[a, c, e]* Darya Botkina,[d, f] Karim Elgammal,[a, c] Assel Ten,[f] Håkan W. Hugosson,[a] Anna Delin,[a, b, c] Valentina Yu[e, f]

[a] Department of Materials and Nano Physics, School of Information and Communication Technology, KTH Royal Institute of Technology, Electrum 229, SE-16440 Kista, Sweden
[b] Department of Physics and Astronomy, Materials Theory Division, Uppsala University, Box 516, SE-75120 Uppsala, Sweden
[c] Swedish e-Science Research Center (SeRC), KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden
[d] Department of Production Engineering, School of Industrial Engineering and Management, KTH Royal Institute of Technology, Brinellvägen 68, 10044 Stockholm, Sweden
[e] Kazakh-British Technical University, Department of Chemical Engineering, Tole bi 59, 050000 Almaty, Kazakhstan
[f] Institute of Chemical Sciences, Walikhanov str. 106, 050010, Almaty city, Kazakhstan
E-mail: aminami@kth.se

DOI: http://dx.doi.org/10.3998/ark.5550190.p009.452

Table of Contents

1-(3-hydroxypropynyl-1)cyclohexanol

25
GEOMETRY FILE / created by CPMD

C	4.866453951753	9.263434266246	5.279589899064
C	6.045884693986	8.538890761873	5.723033581710
C	7.017516028313	7.928477052544	6.097080814450
C	8.198520218280	7.191952213252	6.552714856199
C	7.787629027972	5.900724905628	7.323932617368
C	7.712688985637	4.688320482235	6.386308548451
C	9.093162178797	4.371111401939	5.752627439565
C	9.986420405024	5.629671943915	5.600274731844
C	9.141937885437	6.882233745157	5.348839524855
O	4.025858994510	8.357942154160	4.510022786353
O	8.920978264122	8.014641232173	7.522332472009
H	3.223563814585	8.849097442081	4.254035629422
H	5.163987159524	10.126526403519	4.660614541567
H	4.313391662837	9.649518361146	6.152043794385
H	9.038196979777	8.897660453964	7.124591141172
H	6.832123486101	6.073674064250	7.829974284869
H	8.542865327896	5.735684587271	8.103884905500
H	6.970601051106	4.888267671878	5.600592252952
H	7.341906285574	3.815092728413	6.937723487844
H	8.939091875802	3.903832280470	4.770560605679
H	9.622734504485	3.629983778171	6.366365039166
H	10.698323130592	5.487403139367	4.776938014195
H	10.589001978920	5.779628546847	6.506253101587
H	8.542108901139	6.753615991927	4.437820148424
H	9.775994869097	7.764191044345	5.187070576918

Total energy = -91.20380634 A.U.

1-(4-hydroxybutynyl-1)cyclohexanol
28
GEOMETRY FILE / created by CPMD

C	10.599124737129	9.405222677137	6.682582730640
C	10.541573142326	7.955094560351	7.193806194012
C	9.262551985020	7.331474420674	6.855651148537
C	8.195651375423	6.845862803855	6.563330504405
C	6.911377470784	6.228710023554	6.218780913735
C	7.085280421349	5.185558386469	5.071162881906
C	7.367320610923	3.784925102121	5.617539710050
C	6.189981874777	3.263869935336	6.485860798348
C	5.373241865550	4.403524448833	7.147848602466
C	6.264142106255	5.600240323819	7.496068505337
O	11.887542703387	9.961738760168	7.043560908522
O	6.048506221076	7.300960976515	5.723288376249
H	11.921097090164	10.879713120002	6.722384650868
H	10.464265417105	9.414943491662	5.590911398016
H	9.784067516491	9.987181721355	7.137423312030
H	10.697103205884	7.952623674643	8.282491239334
H	11.373950278161	7.387460762112	6.752798095703
H	6.155939677522	5.175548918853	4.482330942692
H	7.878342579842	5.527303252836	4.397744092713
H	8.291431775085	3.816015915555	6.211608916516
H	7.560453229257	3.089368237580	4.790924179604
H	6.584829697813	2.596610768661	7.263654347058
H	5.515932308891	2.652199441214	5.871006654963
H	4.873500354228	4.032345145746	8.051858064841
H	4.563393663050	4.724257327613	6.473877864375
H	7.053342915506	5.280791590233	8.188645351478
H	5.703484145324	6.397272042163	7.999159257005
H	5.174402181750	6.904748584684	5.548620125742

Total energy= -98.06663377 A.U.

1-(2-ethoxyethyl) -4-(4-hydroxybutynyl-1)piperidine-4-ol

40
GEOMETRY FILE / created by CPMD

C	18.425684014156	7.893258504541	5.899364048487
C	17.900197155554	6.651163177688	6.639923518944
C	16.443772588129	6.566722926304	6.547609482984
C	15.240658099079	6.529211501704	6.451185789450
C	13.782796169550	6.465087218445	6.344213039330
C	13.339727822547	5.191432739474	5.562543263270
C	11.939866601250	4.714917079480	5.984273099445
C	11.582660125366	6.468503260298	7.647825084044
C	13.126022901813	6.482226297037	7.743702497057
C	9.676725436654	5.434009912464	6.498412352859
C	8.708097674853	6.594727570519	6.727147280198
C	6.386688862700	7.093295516320	6.918513777203
C	5.011891725861	6.445579329754	6.929308788346
N	11.087238405286	5.857122580756	6.380954915036
O	19.868613451195	7.920195759333	6.027975734413
O	13.345430740893	7.650536538342	5.609335346521
O	7.374555377562	6.058698324774	6.739699074944
H	20.199549943514	8.705694682823	5.558523380143
H	18.131295262516	7.841005673927	4.840798053560
H	17.979864600729	8.797942458961	6.338347922028
H	18.217304900257	6.700407775219	7.691811214879
H	18.366883485928	5.753210369734	6.209355921330
H	13.364462166257	5.450061992509	4.497590940811
H	14.062364037577	4.382402572101	5.719581463665
H	12.014273778446	3.978294811576	6.811366376385
H	11.455409263543	4.197509956670	5.148408229306
H	11.176881412682	5.918821791139	8.520539140019
H	11.197985757746	7.492189446573	7.704738284411
H	13.485299625445	5.614380525187	8.311410969209
H	13.457359617535	7.379177790139	8.277103861809
H	12.395096471402	7.497387128960	5.421894287220
H	9.552502743650	4.699046904135	7.320362205036
H	9.391516934617	4.931687768681	5.566131667559
H	8.813695884752	7.338626259024	5.917683355651
H	8.905369635558	7.106490128820	7.684102080454
H	6.472062408334	7.828128541915	6.098057607622
H	6.579807269200	7.628986239138	7.865430508404
H	4.825941648201	5.918547962822	5.986106133135
H	4.931321576158	5.723027956679	7.749922536603
H	4.232997556374	7.207332875056	7.060143661410

Total energy= -145.08911088 A.U.

1-(2-ethoxyethyl) -4-(3-hydroxypropynyl-1)piperidine-4-ol

37

GEOMETRY FILE / created by CPMD

C	16.524454352199	4.440774115879	7.941345546709
C	15.825469635287	5.533289331406	7.289490115714
C	15.238611177136	6.437611384239	6.747691900291
C	14.544080043739	7.533891939441	6.075453674409
C	13.569388989696	8.242923910342	7.062065587928
C	12.366116040969	8.824301506045	6.311646048418
C	12.357571249973	6.625487232438	5.149221817357
C	13.787105255484	7.032744606708	4.811648605953
C	10.390324541011	7.365075126777	6.408611434958
C	9.405644731203	6.484621280122	5.620443545293
C	8.327046167030	5.222379226453	7.368881320856
C	6.975890333637	5.048764725688	8.042577697207
N	11.555972307018	7.784763423580	5.617110466505
O	16.032590225407	3.183269172122	7.398330488029
O	15.525870603901	8.530464330876	5.657114157039
O	8.197402978480	6.256154216201	6.370578782563
H	16.517171914999	2.462037076802	7.840557515738
H	17.609630107533	4.536138246241	7.768600108117
H	16.353477004234	4.479765439397	9.030132828015
H	16.191892316578	8.071732178546	5.111755373729
H	14.129153196853	9.026523768610	7.586587760363
H	13.234573500589	7.519975612103	7.814885015756
H	11.710676936584	9.362491439026	7.005291098977
H	12.719047844235	9.562261717749	5.577705405402
H	11.878142625746	6.192195823639	4.262402622731
H	12.388251256010	5.823058980198	5.916149793638
H	13.782997466690	7.853173892320	4.083132315746
H	14.324565384446	6.187943915224	4.365629186976
H	9.842499598652	8.263821110850	6.717024251198
H	10.697963385280	6.830383474759	7.333159287321
H	9.853360670714	5.517354322819	5.341069064882
H	9.105264546408	7.002733692829	4.701728342599
H	9.094397280163	5.493836052754	8.111456813094
H	8.651231567705	4.284832521521	6.882116142390
H	7.031158739380	4.266550235716	8.810399698739
H	6.661534037221	5.983211375529	8.522440570684
H	6.211518853895	4.764281189603	7.309875511318

Total energy= -138.25966720 A.U.