

Supplementary Materials: Investigation of the Structures and Energy Landscapes of Thiocyanate-Water Clusters

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xyz files for structures pictured and discussed in the text

Putative Global Minima for $\text{SCN}^-(\text{H}_2\text{O})_{3-50}$

14

waters = 3 energy = -42.8891074847
S -0.508424977536 -1.4845140077 -1.36429945815
C 0.629515104984 -0.652792225442 -0.628479340509
N 1.52412208809 0.00107710022476 -0.0500044052591
EP -0.961449420996 -1.16467943936 -1.02522026014
EP -0.0554005340757 -1.80434857603 -1.70337865616
O 0.116893467755 0.319795227155 2.45565338464
H -0.736210613859 0.230456205345 2.03084306801
H 0.749065459074 0.0856745611348 1.7761109451
O 0.141743012629 2.4014371238 0.615447576381
H 0.689929208904 1.80369471555 0.107089683151
H 0.144525026241 2.03592319283 1.5001077748
O -2.01040690841 0.610402370735 0.668686577261
H -1.76055010899 -0.0760770147852 0.0501807381309
H -1.41496239768 1.33481991496 0.476600929021

17

waters = 4 energy = -56.7500792444
S 0.162021644999 0.218972601771 1.54121711936
C -1.04430483256 0.292341238693 0.508021362179
N -1.99267470486 0.350020984701 -0.304239453211
EP 0.572007475084 0.0906583097792 1.05341894224
EP -0.247964185086 0.347286893763 2.02901529648
O -0.591394842223 0.533664929353 -2.76712958729
H -0.810404572573 -0.39521297665 -2.84097004877
H -1.0800172303 0.835297095253 -2.00129798807
O 1.73943746771 0.0954813749672 -1.36943081511
H 1.43829052774 0.262092066445 -0.476243691361
H 0.994670174436 0.332668108509 -1.92196676173
O 0.870751129517 -2.3802507706 -0.592969054711
H 0.603618058787 -2.04811459443 0.264094141909
H 1.31305499533 -1.64071591586 -1.0097271727
O -1.49605514896 -1.95234852615 -1.93452956479
H -0.692806502785 -2.23591387741 -1.49793576733
H -1.84794919809 -1.26609923447 -1.36755132195

20

waters = 5 energy = -69.2452492596
S 0.90241466409 -0.462799528288 2.18347884562
C 0.290307696571 0.497932192162 1.07423603107

N -0.19090847286 1.25322442522 0.202189793209
EP 1.1594044595 0.0513465434628 2.48697524091
EP 0.645424868678 -0.976945600039 1.87998245032
O 0.143782587218 -0.574588326932 -1.98712188135
H 0.199013321943 0.00723987728575 -1.2290603095
H -0.72353784622 -0.406851975328 -2.35570243169
O -2.3301341037 0.341732665866 -2.71002128671
H -1.88782224469 1.18481944945 -2.61104283086
H -2.58862870031 0.100451385295 -1.82052945022
O -0.53831160279 2.39772407246 -2.31041027813
H -0.45377232375 2.22340152478 -1.3730220983
H 0.121089778976 1.83708672611 -2.71919802699
O -2.58365637723 -0.323904583867 -0.0783573155015
H -1.95160251183 0.343469874151 0.188758921409
H -2.11015523537 -1.15125652472 0.00834490261855
O -0.69974406049 -2.35655005874 -0.0100352180415
H -0.31377171472 -1.92009033102 -0.769482447531
H -0.21466077224 -2.00931603209 0.738533131679
23

waters = 6 energy = -82.9357375127

S 0.759969060364 -0.160931268994 1.80534061152
C -0.295987800896 0.554259039049 0.855836567059
N -1.12614256604 1.11651557053 0.109371123298
EP 0.83926980282 0.393686721802 2.13490134421
EP 0.680668317907 -0.71554925979 1.47577987883
O 0.119906506933 -2.47167708375 -0.411391700222
H 0.363391511865 -1.95081569362 0.353886226178
H -0.769559029416 -2.18752636211 -0.621965362032
O 1.35719948605 -0.957295215152 -2.32898706377
H 1.01827241513 -1.5694544696 -1.67582450531
H 1.89404857835 -0.343897427952 -1.827222132
O -0.838204179516 0.592303584652 -2.65121886724
H -0.0619990106844 0.032391035432 -2.63587894883
H -0.996023435086 0.80896515242 -1.73231588671
O 2.57917501573 0.987965771766 -0.827646973312
H 1.9795834663 1.69589201031 -1.06336344421
H 2.30275994671 0.721293124112 0.0491153939277
O 0.574137504912 2.74773108986 -1.51490818941
H 0.0265793625306 2.5049350482 -0.768274408462
H 0.22272859212 2.23910242919 -2.24568893735
O -2.27065770491 -1.25231622909 -1.08688170083
H -2.15192173734 -0.56394511769 -0.432451549492
H -1.97468950407 -0.857364092624 -1.90703258572

26

waters = 7 energy = -95.1650247976

S 0.912631943323 -1.25379868215 -1.02776854672
C 0.934555387615 0.145244580186 -0.272588228718
N 0.951790799793 1.24512135875 0.321106989839
EP 1.30287687266 -1.5054343398 -0.572918691353

EP 0.522387013985 -1.00216302451 -1.48261840209
O -1.64353789115 1.78931800477 1.24531116842
H -2.17128827572 1.18455567042 0.723800007909
H -0.744101258167 1.63189763792 0.958144994669
O -2.97967324537 0.00839314738588 -0.290892921183
H -2.6329496213 -0.795406492161 0.0963030343292
H -2.54192818796 0.0741820556359 -1.13958775695
O -1.01589611422 -0.276598899373 2.97007758693
H -1.31291260009 0.515144058536 2.52157325505
H -0.0626764057917 -0.193744191014 2.99726443628
O -1.68172215672 -2.04022575912 0.977766972809
H -0.887525072177 -2.03337415182 0.443504971179
H -1.45997092417 -1.51135602901 1.74415789097
O -0.768829935427 2.80065133353 -1.3118683984
H -1.38869699671 2.81094913266 -0.582560081108
H 0.0322530335623 2.43082537371 -0.940752949721
O -1.47351994392 0.416520184336 -2.53622904174
H -0.734383019037 -0.138314835054 -2.28709745495
H -1.22183878451 1.2944745296 -2.24972493769
O 1.71605346861 -0.0734948048641 2.69938824893
H 1.58070537645 0.532069243626 1.97055018933
H 1.96455101642 -0.898684317892 2.282803232
29

waters = 8 energy = -108.984635841

S -0.466433650711 -0.822880846219 -1.49983307817
C -0.67160970239 -0.529355623477 0.0493104695478
N -0.83291162981 -0.298596800566 1.26719061712
EP -0.643969479289 -0.213247178542 -1.63885761128
EP -0.288897822133 -1.4325145139 -1.36080854507
O -1.27232960089 2.50473127497 0.978030470568
H -1.18860976893 2.57005411687 0.0267388454278
H -1.30700336822 1.56408728006 1.15186500309
O 1.42324061911 2.49353548319 1.33713009389
H 0.47358720793 2.61073897329 1.31156487267
H 1.55816018094 1.75676055979 1.93310934191
O 1.62019324134 0.0523615812541 2.58569644645
H 2.23031614662 -0.176778711181 1.88464252068
H 0.753860597489 -0.0365281355209 2.18845822013
O 1.97496498665 1.4238270238 -1.09352201061
H 1.80886746425 1.82993376457 -0.242804214772
H 1.26803923894 0.786903448611 -1.19752290761
O 0.543965773539 -2.55906628155 2.38464540588
H 1.13701629072 -1.90753074624 2.75884370933
H -0.192849562381 -2.04833751735 2.0492484319
O 3.16427825718 -0.581395866268 0.449104209888
H 2.92543085651 0.0693140373591 -0.211017279322
H 2.74957961012 -1.39044963332 0.149623201898
O -0.653952219884 2.43435061298 -1.71979174519
H 0.302225989604 2.47490610136 -1.70217572797

H -0.852462669731 1.50710351064 -1.85032240249
O 1.70385666287 -2.83987770367 -0.109661619062
H 1.00981534828 -2.47645958082 -0.659630492396
H 1.31481179858 -2.89398341315 0.763234998968
32
waters = 9 energy = -121.270945729
S 0.367660062249 1.64817647886 -0.430056364396
C 0.733492792573 0.564954610015 0.674885623334
N 1.02109714031 -0.286634909525 1.54355070803
EP -0.169313210053 1.80464335006 -0.098879941548
EP 0.904633334551 1.49170960766 -0.761232787244
O 1.54374705311 -1.46102811423 -3.50039249593
H 1.63743148867 -2.1942029929 -2.89219050331
H 0.651961937056 -1.14366669001 -3.3581501914
O -1.27696201001 -0.320942284355 3.18946118668
H -1.44620422708 -1.21863546962 2.90356635095
H -0.396001755691 -0.128811065765 2.86817243003
O 0.847296273372 -2.74045420411 -0.947165764454
H 1.66653241758 -2.38753976854 -0.599983706752
H 0.302432360468 -2.88718111954 -0.173973441223
O 3.06530847286 -1.51900633538 0.018068063071
H 3.19131719461 -0.848837991235 -0.653667027982
H 2.53198650901 -1.09048323802 0.687521181594
O -0.726676873561 -2.47469804758 1.30544260015
H -1.45354610149 -2.08431562485 0.820164814224
H -0.102762534752 -1.75800557891 1.42083169488
O -2.6523992274 -1.22035613517 -0.130823442214
H -2.70336148562 -0.353446589485 0.27179613984
H -2.16747012043 -1.07919744235 -0.943934642883
O 2.97466248516 0.350883402155 -1.98003570368
H 2.52314628681 -0.198971815375 -2.62036702603
H 2.28194252919 0.88528951896 -1.59173040508
O -0.805215147921 -0.898617786455 -2.15022378397
H -0.264456149596 -1.55450107688 -1.71019122259
H -0.508830714433 -0.0626084647354 -1.79039532265
O -2.47018749387 1.16674651949 1.18444763109
H -2.1212751558 0.753407228118 1.97415811636
H -1.70326888493 1.54026136979 0.750219184454
35

waters = 10 energy = -135.008524695
S 0.819297664267 1.49397614855 0.62120268057
C 0.492611429433 0.792313469681 -0.76769817588
N 0.235782628462 0.240691866793 -1.85960136491
EP 0.273707364131 1.84394962268 0.572728029435
EP 1.3648879644 1.14400267442 0.669677331706
O -2.24234610265 2.51981293055 0.134610044003
H -2.27426599126 2.26835438359 -0.78841842786
H -1.32234574613 2.41936630953 0.379031115765
O -3.43109370453 0.258843485823 1.13698566394

H -3.07166153592 1.11436764014 0.902211777956
H -2.67590677702 -0.242586778417 1.44438155629
O 1.22341228855 -2.71025428487 1.67616571929
H 1.12490306545 -3.16361495427 0.838913143057
H 0.395049275514 -2.24599044556 1.79660510717
O -1.32620311409 -1.92781126592 -1.05341291174
H -2.21910245122 -1.63613836303 -1.2375040073
H -0.768756955093 -1.24925252107 -1.43425887746
O 2.43268828146 -1.60673108392 -1.79765351959
H 2.79619194609 -1.35602411274 -0.94839328833
H 1.77111564782 -0.939920751087 -1.98182048312
O -1.06409987808 -1.1317686804 1.54765271159
H -1.16899660604 -1.45581737088 0.653102007239
H -0.504996616973 -0.359872577947 1.45926837787
O -3.69317381243 -0.637373912747 -1.42845279194
H -3.75614072208 -0.360322228117 -0.51439077417
H -3.29232670591 0.106757555313 -1.87769859931
O -2.18137691121 1.46731573109 -2.45639623531
H -2.09081265704 1.95598320479 -3.27446350394
H -1.32621343261 1.05764642404 -2.3256356765
O 0.85520885743 -3.63967745665 -0.87062200004
H 0.00112384517187 -3.22938215256 -1.00637322575
H 1.47841344773 -3.03604853466 -1.27494860461
O 3.07212973122 -0.886030863387 0.76835640071
H 2.51372426333 -1.53783114404 1.19211525616
H 2.56530610774 -0.0748949788369 0.806042359363

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waters = 11 energy = -145.851100117

S -0.00374245012284 -2.01729447274 0.284210261491
C -0.497564032883 -0.847268108515 1.24091217505
N -0.885788547631 0.0725639388351 1.99303632092
EP 0.583487503489 -1.74082463482 0.249204400551
EP -0.590972403735 -2.29376431067 0.319216122431
O -0.161741973518 2.39151780411 -0.555187536236
H -1.05420856284 2.40943567081 -0.2096239719
H 0.38313265589 2.16649172894 0.198938941034
O 2.14358695567 3.20967701323 -1.93190617373
H 2.77154082025 3.09620471985 -1.21844291428
H 1.28702755509 3.11890079871 -1.51441663834
O -0.455360370661 0.179725683795 -2.15235601495
H -0.269885164142 -0.545752711175 -1.55610783994
H -0.35974421473 0.964422626175 -1.61259671735
O 2.19548372926 0.605196141835 -2.74798702569
H 1.25906944674 0.407147942935 -2.75969353726
H 2.23879354567 1.55270404885 -2.61920478329
O -3.29164312231 -2.15055622619 0.0436489127351
H -2.3635558253 -2.3610763718 0.146445203578
H -3.51551823944 -1.66012377054 0.834589984103
O -2.59664257701 1.79528672113 0.578722832201

H -2.85393238412 1.24518443162 -0.161156391888
H -2.02267913719 1.23780771942 1.10409410322
O -3.13377716986 0.117064228775 -1.47463199187
H -3.24333541868 -0.735820787005 -1.05413706921
H -2.27171140527 0.0717753353651 -1.88818171518
O -3.67437411758 -0.406689553355 2.15815489007
H -2.74317510011 -0.393802278995 2.37936553183
H -3.82589373478 0.424943068225 1.70908827104
O 2.67765654824 -0.181916695275 -0.190897302006
H 2.56888049875 0.00920108456509 -1.12249464275
H 2.0691048842 -0.900909074355 -0.0207600896459
O 1.43365659093 1.59805696739 1.49768357975
H 1.87671608593 0.921246298335 0.985963497921
H 0.69854771996 1.14443623443 1.91008510553
O 3.74831305013 2.49667203378 0.190376305858
H 3.82395925995 1.56704841371 -0.0248199207689
H 3.07699983462 2.5314060797 0.871818858632

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waters = 12 energy = -158.002524214

S 0.604445021712 -1.70526454408 1.19342048534
C 0.836016698949 -0.472942525593 0.2157410895
N 1.01806990432 0.495864092717 -0.552874787732
EP 0.714494655993 -1.31992781854 1.70518672684
EP 0.494395387431 -2.09060126962 0.681654243832
O -0.802710486208 -2.97638960197 -1.50404121687
H -0.760001523078 -2.17309877022 -2.02282019108
H -0.220491937675 -2.81398067087 -0.761830504982
O -1.16432144283 1.81076688142 0.761992618393
H -1.19848354728 2.67153281517 0.344683622657
H -0.406264311458 1.38162521341 0.365232420844
O 1.15143610212 2.8631234197 -2.06875739607
H 1.23341296878 2.02540980954 -1.61296408689
H 1.59678179896 3.4906665336 -1.49946951591
O -2.95695808109 2.80076331042 -2.37351867126
H -3.13324399327 1.97801201856 -1.91719046819
H -2.29566782329 2.57537099452 -3.02783154662
O -0.803630561878 1.99838381917 -3.87748168213
H -0.797131433108 1.08585873565 -3.5885395196
H -0.0452352392656 2.39210142128 -3.4461409532
O -2.82260248951 0.414409472767 -0.890010831422
H -2.33507379596 0.898560193347 -0.223568266212
H -2.96303225038 -0.450133329023 -0.503905837772
O -2.74549137305 -2.08943763558 0.195554313835
H -2.21099097583 -2.52641856261 -0.467460644352
H -2.17018997536 -2.01534417655 0.9569808048
O 2.1468705364 2.28909370456 1.42479149561
H 2.05769531681 1.62392088575 0.742277948975
H 1.61369337553 1.96233383402 2.14948587404
O -0.794282043798 -0.402098611593 -2.53728315664

H -1.57187971064 -0.152721430603 -2.03789880552
H -0.0593254075246 -0.158818375833 -1.97435748687
O 0.287996063392 1.06207740875 3.04641036282
H 0.454166890086 0.160907366277 2.76980296795
H -0.381799110304 1.37940381551 2.44067922043
O 1.73567797623 4.5777082573 -0.0214714547018
H 0.792553504979 4.71562834487 0.0664269023182
H 1.93286199934 3.86969282966 0.591769489182
O -1.03125003135 3.99383025954 -0.841610978652
H -0.30748785291 3.63200869695 -1.35296731811
H -1.8156075233 3.7635031896 -1.33957142454

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waters = 13 energy = -171.831151622
S -2.26503369155 1.32632199312 -0.13562766982
C -0.899357640757 0.636997766693 -0.569057058725
N 0.174287053263 0.0950762050363 -0.909803433651
EP -1.99511319624 1.91204675868 -0.216679660668
EP -2.53495418685 0.740597227553 -0.0545756789726
O 1.72673516158 2.42669275989 -1.41489041278
H 1.91484023962 2.54587607316 -0.483953434544
H 1.14500053239 1.66722329537 -1.44687155829
O 1.07260212759 0.134512719026 1.77266281669
H 1.92386135958 -0.299498157004 1.71588148656
H 0.751760787593 0.152469437386 0.87101419843
O -0.392312556827 -2.15678128496 2.06137818189
H 0.0377744329029 -1.30241232627 2.09758182372
H -0.481443802527 -2.34116285011 1.1263429422
O 4.41517019959 1.41063642551 1.0774292215
H 4.44566020797 1.34532408014 0.122946902687
H 3.69080997552 2.01096848063 1.25388184796
O 1.9026242734 2.69947502942 1.30661337111
H 1.5489640243 1.87333926733 1.63624342252
H 1.13087095737 3.23756873463 1.13030732011
O -0.852235765607 -2.54936589204 -0.617961725139
H -0.567659186167 -1.68488748877 -0.91448339502
H -1.74890067378 -2.41470687483 -0.311219436664
O -3.001322117 -1.7079912954 0.850871923951
H -2.98427596427 -0.792724413914 0.57117958527
H -2.39502100304 -1.74418987476 1.59068302286
O -0.237030220907 3.89472940812 0.0230294532349
H 0.267081700003 3.65193448413 -0.753600211455
H -0.986557723947 3.29939837894 0.0184112399059
O 2.03086154819 -3.49416235376 1.89756942176
H 1.18280816283 -3.11635542575 2.1305913536
H 2.62929759214 -2.74733249365 1.87882638734
O 4.08257631781 1.0350005861 -1.61839947136
H 3.32285894914 1.60743970071 -1.72505227168
H 3.72260080872 0.148882548576 -1.65640337173
O 2.59055714377 -1.31018954841 -1.26300467416

H 2.34796854456 -2.23593272876 -1.24345536302
H 1.75502421531 -0.843173664324 -1.26657251298
O 3.41873021755 -1.11762843727 1.33118537077
H 3.23508977526 -1.24102971768 0.399906598356
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59

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62

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74

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77

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86

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89

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98

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104

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107

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116

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143

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146

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Low Energy Minima for SCN⁻(H₂O)₁₀

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EP	-0.545590300136	0.34997347413	-0.0484746511355
EP	0.545590300136	-0.34997347413	0.0484746511355
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H	-3.09356365553	0.774378235035	-1.40962110843
H	-2.1416434104	0.925390160974	-0.242171564805
EP	-2.94795875246	0.980788674805	-0.573462571089
O	-4.2503913688	-1.23513266273	0.51578298337
H	-3.89095920019	-0.379608508411	0.281009097386
H	-3.49520444129	-1.73656292697	0.823178875721
EP	-4.10770667676	-1.18980437271	0.52507947636
O	0.404114624279	-4.20423043342	1.05496303872
H	0.305605401182	-4.65759110282	0.217710462487
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EP	0.285463795462	-4.20283469613	0.963202302353
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H	-3.03840011549	-3.13011451158	-1.85870668787
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O	1.61339061719	-3.10070723247	-2.41885620016
H	1.97689428182	-2.85000026129	-1.5695959689
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EP	1.575234193	-2.98325394783	-2.33371623763
O	-1.88339754235	-2.62574482895	0.926450031021
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O	-4.5124714767	-2.1313500613	-2.04965547251
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H	-4.11162437018	-1.38721859324	-2.49890127988
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O	-3.00067457548	-0.0266604174672	-3.07759891588
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H	-0.818173819095	-4.72335830111	-1.62757590632
H	0.659115783467	-4.53002468321	-1.89615128518
EP	0.0063557136109	-5.0038590714	-1.56096115886
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H	1.74600844347	-1.56887112739	0.184839678793
EP	2.1164698914	-2.35961013228	0.206224223617

45

-134.953967633

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N	-0.960521484325	-1.11667461179	-2.42817550633	
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O	-4.52221611156	0.783060215766	-2.85153674972	
H	-4.49554888058	1.20330180062	-1.99193352198	
H	-3.67902782189	0.998349102802	-3.25017950117	
EP	-4.41086411022	0.86441578376	-2.79252824733	
O	-0.0133509181733	-3.17076437565	0.816883232122	
H	0.17988554595	-2.2410479305	0.696389080604	
H	-0.0958266153154	-3.51591925356	-0.0721036685918	
EP	0.000827796314439	-3.09593344239	0.68765747818	
O	-0.584109292607	-3.88760961174	-1.77182321053	
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EP	-0.705833177856	-3.80298660425	-1.79467583319	
O	-3.2223306881	-0.679998420747	0.673554389577	
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H	-1.72156829849	-3.28664922848	1.35163158017	
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H	-3.54646028792	-3.3978621127	-1.43190770143	
H	-3.09385667066	-4.03291013166	-0.134310240333	
EP	-3.24086840373	-4.0887975813	-0.993514116213	
O	-1.88620617957	1.19603438022	-3.66108652886	
H	-1.39931577416	1.33587400541	-4.47325304649	
H	-1.53105854161	0.381332974454	-3.30560992668	
EP	-1.77841515094	1.10964393019	-3.71954834794	
O	-4.04136282276	1.77234280537	-0.352964790083	
H	-3.18918558997	2.15336498296	-0.564738027535	
H	-3.83382894512	0.984938063812	0.150180618926	
EP	-3.90570701535	1.72032093423	-0.315665636757	
O	-1.57073793012	2.57106799048	-1.24539200359	
H	-1.6452738523	2.21114129842	-2.12920703664	
H	-0.968547396808	1.97878424539	-0.795060606852	
EP	-1.50319177381	2.44917356623	-1.30088313896	
O	-3.64676458503	-1.59821348939	-1.86989416502	
H	-4.09901261529	-0.853223025857	-2.26573853894	
H	-2.73851389959	-1.50853177655	-2.15845910188	
EP	-3.58839074355	-1.49136538061	-1.95750681411	

45

-134.803844584

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H	-1.04325724162	-1.59638930252	-1.52277766301	
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H	-3.81228043116	-1.89931606271	1.8949657675	
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EP	-3.31094423409	-1.32444572099	2.32058680167	
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H	-1.46308327344	-3.38713517891	0.982594240646	
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H	-0.344827405278	-5.05716757356	0.2387956676	
EP	0.503612041714	-5.26418519544	0.254962486428	
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45

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EP	2.86916512292	-3.13189926689	-1.33717236359
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H	-1.58980288405	-1.64613910465	-5.70214542021
EP	-1.39479930669	-2.4926597389	-5.79348860619
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H	0.257423847624	-2.34104729061	-0.225426979894
EP	0.273374415807	-3.12102618833	-0.61829547634
O	2.11431556754	-0.231225110014	-3.74227541849
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Low Energy Minima for $\text{SCN}^-(\text{H}_2\text{O})_{13}$

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EP	1.33444323509	−3.74778624087	−0.481025692828	
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57

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-171.120218928

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