Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Encapsulation of Astatide by a water cage

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Supplementary information

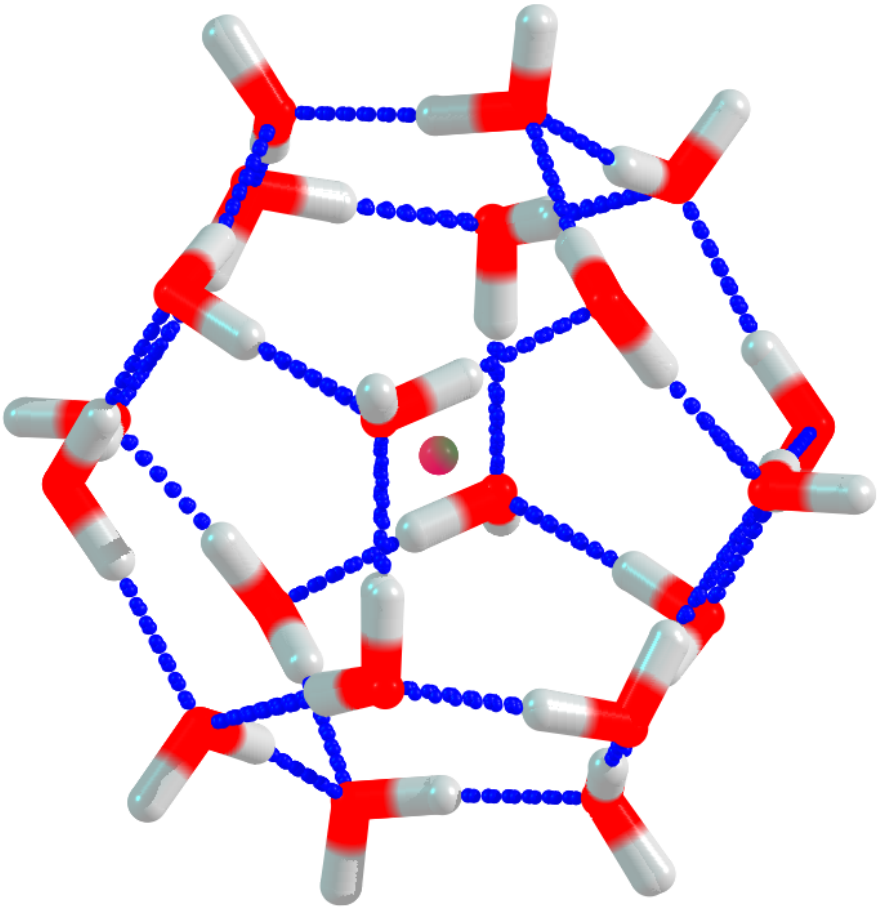

Figure S1: Virtually identical geometries whose differences are shown as shadows and color changes are obtained via our standard DFT calculations and scalar ZORA and spin–orbit ZORA calculations with WB97X and the TZ2P basis set.

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61
system s512_at_def2tzvppd2_optimized
O 1.050049   0.609907   3.747588
H 0.129497   0.343907   3.562489
H 1.176012   1.434915   3.215649
O -1.144223   3.592943   1.011393
H -1.361396   4.526947   1.102416
H -1.028711   3.450564   0.028521
O 1.435067   2.922150   2.235643
H 0.564280   3.047623   1.810576
H 1.989101   2.535511   1.530831
O -1.717703   -0.250175   3.458652
H -2.159126   -0.487237   4.281412
H -1.748711   -1.059923   2.899787
O -3.131545   1.782066   1.924709
H -2.616904   1.093874   2.386647
H -2.444860   2.398402   1.593401
O -1.964100   -2.632826   2.007101
H -2.458969   -3.368224   2.384126
H -2.441736   -2.389561   1.166948
O -3.988155   0.509971   -0.380489
H -3.658880   0.975326   0.431317
H -3.422934   0.832154   -1.114567
O -3.347668   -2.020016   -0.228765
H -3.550068   -1.021810   -0.265195
H -4.188345   -2.457637   -0.398510
O 2.506215   -1.338897   2.645748
H 3.056540   -1.595194   3.393312
H 1.937161   -0.581212   2.988794
O -0.809942   3.395062   -1.670419
H 0.096072   3.033290   -1.712963
H -1.375758   2.650411   -1.969052
O 3.986541   -0.501566   0.382589
H 3.658606   -0.967001   -0.429771
H 3.421762   -0.826087   1.116215
O 1.964097   2.631588   -2.009145
H 2.457248   3.368786   -2.384860
H 2.439630   2.390325   -1.167059
O 3.342432   2.027281   0.231772
H 3.544387   1.028757   0.268747
H 4.185893   2.463784   0.390483
O 0.812729   -3.395569   1.670813
H -0.092607   -3.032330   1.712341
H 1.379701   -2.651994   1.970311
O -2.506269   1.339410   -2.648191
H -3.053187   1.599538   -3.396999
H -1.939864   0.579733   -2.991417
O 3.136772   -1.776598   -1.923906
H 2.615240   -1.091991   -2.383751
H 2.456108   -2.399236   -1.592435
O 1.710128   0.245109   -3.458268
H 2.161665   0.483283   -4.275250
H 1.739708   1.052623   -2.896480
O 1.153299   -3.593680   -1.007053
H 1.350538   -4.531376   -1.104665
H 1.037238   -3.455066   -0.023299
O -1.056070   -0.614457   -3.750151
H -0.135469   -0.344889   -3.570574
H -1.177207   -1.435581   -3.210858
O -1.425709   -2.915346   -2.220303
H -0.553589   -3.036859   -1.796595
H -1.978931   -2.526002   -1.516397
At -0.000667   -0.001899   -0.002214
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