**KE07 Kemp Ring-Opening**

Starting point: "Supplementray Data1\_KE07.pdb" (sic)

Chain letters "A" and "B" added using a data-set named "KE07 Add Chain Letters.mop" and the following keywords:  
 "**geo\_dat="Supplementray Data1\_KE07.pdb" 0SCF residues0 PDBOUT XENO=(B254=LG1)**"

Keywords used:

|  |  |
| --- | --- |
| Option | Purpose |
| 0SCF | Stop the run after the chain letters have been added |
| RESIDUES0 | Create PDB label, but keep the original atom names. |
| PDBOUT | Output geometry in PDB format, so all PDB data are preserved |
| XENO=(B254=LG1) | Substrate 254 was not recognized, so explicitly re-define it. |

Hydrogenation done using a data-set named "KE07 Add-H.mop" and the following keywords:

|  |  |
| --- | --- |
| Option | Purpose |
| ADD-H | Add hydrogen atoms to form a neutral system. |
| SITE | Modify the hydrogenated system to create charged sites. |
| HTML | Generate a web-page so the effects of adding hydrogen atoms can be examined graphically. |
| OUTPUT | Minimize output. |
| MOZYME CHARGE=0 GNORM=5 NOOPT OPT-H CVB | These keywords will be used in later jobs, but they are defined here to minimize the chance of forgetting to add them later. |
| GEO\_DAT | Geometry read in from "KE07 Add Chain Letters.pdb" created by the previous run. |

SITE keywords used in specifying ionized groups:

|  |  |
| --- | --- |
| Option | Reason |
| SALT | Form salt bridges between residue pairs that are within 4 Å. |
| "[LG1]254:B.N2"(0) | By default, a hydrogen atom would be assigned to the ring nitrogen in the substrate. This atom would be deleted by this keyword. |

Chorismic acid PDB ligand: ISJ

Prephenic acid PDB ligand: PRE