In[1]:=

$$\text{BB}[1] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix};$$

$$\text{BB}[2] = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix};$$

$$\text{BB}[3] = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

$$\text{BB}[4] = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

$$\text{BB}[5] = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}; \ \text{BB}[6] = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

In[5]:=

```
xyzTP[{θ_, ϕ_}] := {Cos[θ] Sin[ϕ], Sin[θ] Sin[ϕ], Cos[ϕ]};
InnerProductMatrix[M_, N_] := Flatten[M].Flatten[N];
```

$$\text{NormMatrix}[\text{M\_}] := \sqrt{\text{InnerProductMatrix}[\text{M}, \text{M}]};$$

$$\text{YRot}[\text{t\_}] := \begin{pmatrix} \text{Cos}[t] & 0 & \text{Sin}[t] \\ 0 & 1 & 0 \\ -\text{Sin}[t] & 0 & \text{Cos}[t] \end{pmatrix};$$

$$\text{ZRot}[\text{t\_}] := \begin{pmatrix} \text{Cos}[t] & -\text{Sin}[t] & 0 \\ \text{Sin}[t] & \text{Cos}[t] & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

```
id = IdentityMatrix[3];
matrixL[L_] := Table[InnerProductMatrix[L[BB[j]], BB[i]], {i, 6}, {j, 6}];
MatrixUbar[U_] := matrixL[U.#.Transpose[U] &];
```

$$\text{ProjToVSigOfU}\left[\begin{pmatrix} \text{a\_} & \text{g\_} & \text{m\_} & \text{q\_} & \text{t\_} & \text{v\_} \\ \text{gdum\_} & \text{b\_} & \text{h\_} & \text{n\_} & \text{r\_} & \text{u\_} \\ \text{mdum\_} & \text{hdum\_} & \text{c\_} & \text{i\_} & \text{o\_} & \text{s\_} \\ \text{qdum\_} & \text{ndum\_} & \text{idum\_} & \text{d\_} & \text{j\_} & \text{p\_} \\ \text{tdum\_} & \text{rdum\_} & \text{odum\_} & \text{jdum\_} & \text{e\_} & \text{k\_} \\ \text{vdum\_} & \text{udum\_} & \text{sdum\_} & \text{pdum\_} & \text{kdum\_} & \text{f\_} \end{pmatrix}, \text{id}, \text{MONO}\right] := \begin{pmatrix} a & g & 0 & 0 & 0 & 0 \\ g & b & 0 & 0 & 0 & 0 \\ 0 & 0 & c & i & o & s \\ 0 & 0 & i & d & j & p \\ 0 & 0 & o & j & e & k \\ 0 & 0 & s & p & k & f \end{pmatrix}$$

(* This is $P(T, V_{MONO}(I))$ in the 2022 paper *);

```
ProjToVSigOfU[Tmat_, U_, Σ_] := MatrixUbar[U].ProjToVSigOfU[
    Transpose[MatrixUbar[U]].Tmat.MatrixUbar[U], id, Σ].Transpose[MatrixUbar[U]];
Alpha[Tmat_, {θ_, ϕ_}, MONOorXISO_] :=
```

$$\text{ArcCos}\left[\frac{\text{NormMatrix}[\text{ProjToVSigOfU}[\text{Tmat}, \text{ZRot}[\theta].\text{YRot}[\phi], \text{MONOorXISO}]]}{\text{NormMatrix}[\text{Tmat}]}\right];$$

(* This is an angular version of the monoclinic distance function *)

This is the cubic example from Section 15.5 of the beachball paper.
Change Tmat to suit yourself, but make sure Tmat is symmetric.

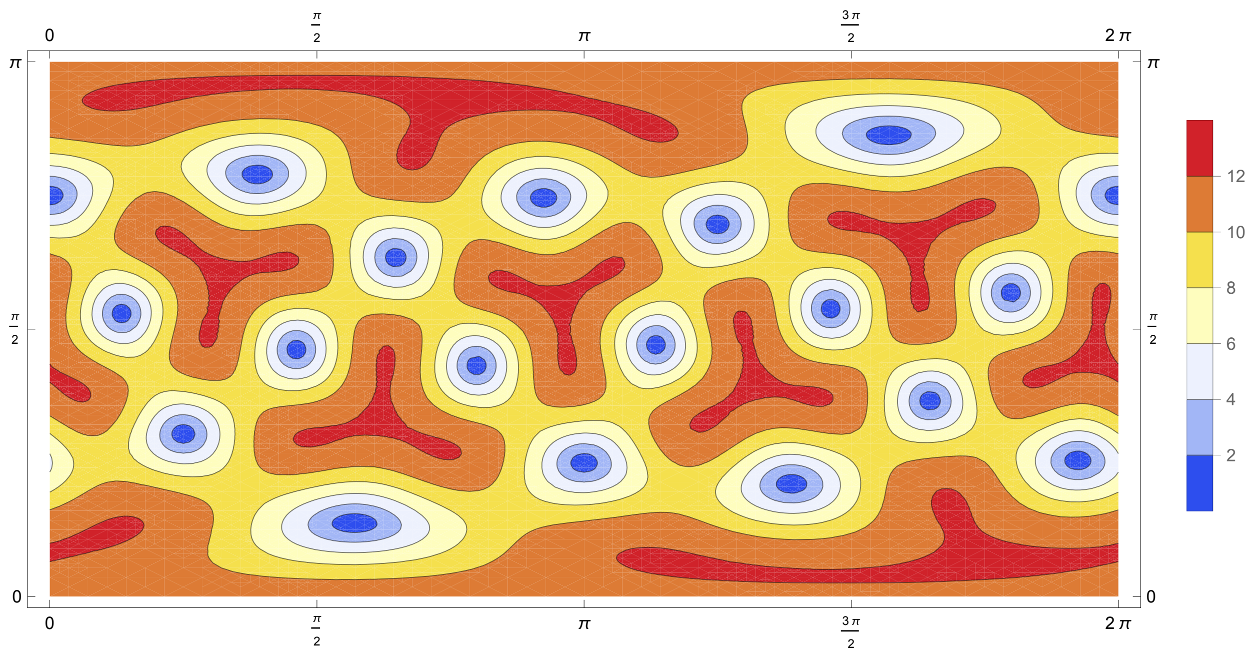
In[16]:=
$$\text{Tmat} = \frac{1}{36}\begin{pmatrix} 52 & 4 & 16 & -6 & -2\sqrt{3} & 0 \\ 4 & 64 & 4 & 12 & 4\sqrt{3} & 0 \\ 16 & 4 & 52 & -6 & -2\sqrt{3} & 0 \\ -6 & 12 & -6 & 45 & 3\sqrt{3} & 0 \\ -2\sqrt{3} & 4\sqrt{3} & -2\sqrt{3} & 3\sqrt{3} & 39 & 0 \\ 0 & 0 & 0 & 0 & 0 & 108 \end{pmatrix};$$

cpMONOprelim will take 10 seconds or so:

In[17]:=
```
Clear[cpMONOprelim]
cpMONOprelim[Tmat_] := cpMONOprelim[Tmat] =
   ContourPlot[Alpha[Tmat, {θ, ϕ}, MONO] / Degree, {θ, 0, 2 π},
    {ϕ, 0, π}, ColorFunction → "TemperatureMap", PlotLegends → Automatic];
```

In[19]:=
```
Show[cpMONOprelim[Tmat], FrameTicks → {Range[0, 2 π, π / 2], Range[0, π, π / 2]},
 AspectRatio → Automatic, ImageSize → 600]
```

Out[19]=



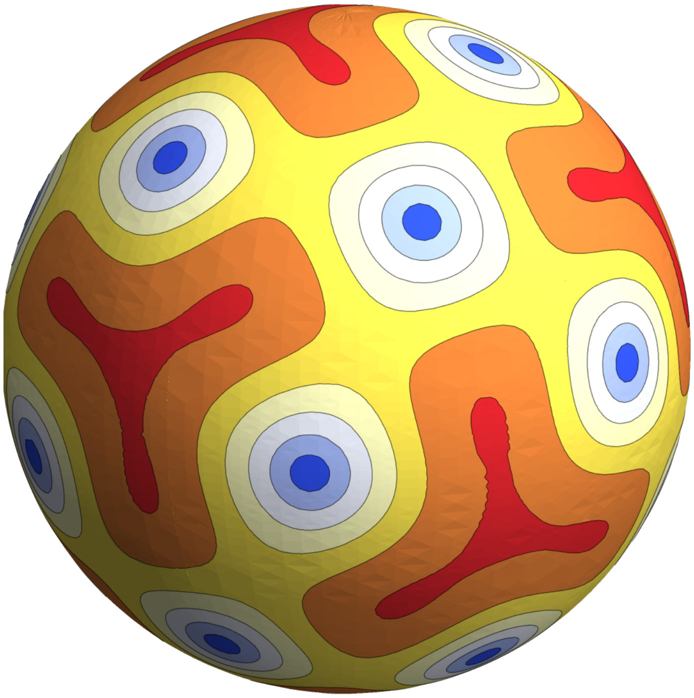
Plot on sphere.

(Note: if the legend is removed from cpMONOprelim, then you have to remove the leading “1,” in the four arguments like “[[1,1,1]]” below.)

In[20]:=
```
eye = 10 xyzTP[{30 Degree, 75 Degree}];
```

In[21]:=
```
Clear[cpMONO]
If[$VersionNumber < 12,
  cpMONO[Tmat_] := Graphics3D[
    GraphicsComplex[xyzTP /@ cpMONOprelim[Tmat][[1, 1, 1]], cpMONOprelim[Tmat][[1, 1, 2]]]],
  cpMONO[Tmat_] := Graphics3D[
    GraphicsComplex[xyzTP /@ cpMONOprelim[Tmat][[1, 1, 1, 1]], cpMONOprelim[Tmat][[1, 1, 1, 2]]]]];
```

In[23]:=
```
Show[cpMONO[Tmat], Boxed → False, Lighting → "Neutral", ViewPoint → eye]
```
Out[23]=



Try a different lighting.

In[24]:=
```
Show[%, Lighting → {{"Ambient", White}}]
```
Out[24]=