1 GFN2-xTB E^Γ

$$E^\Gamma = \frac{1}{3}\sum_A \sum_{\mu \in A} (q_{A,\mu})^3 \Gamma_{A,\mu} \tag{1}$$

where $q_{A,\nu} = \sum_B \sum_{\nu \in B} P_{\mu\nu} S_{\mu\nu}$ is the partial charge of shell μ associated with atom A. P, S are the density and overlap matrices. $\Gamma_{A,\mu} = \Gamma_A K_\mu$ is just the product of an element specific constant and a shell specific constant, for our purposes the element is always carbon and the shell is either the first or second in GFN2 thus we have 2 numbers $\Gamma_{\text{Carbon},1(2)}$ henceforth referred to as $\mathit{\Gamma}_{1(2)}$.

Let us first rewrite the inner expression a bit given our new definition and knowledge of the atoms we are working with.

$$\sum_{\mu \in A} (q_{A,\mu})^3 \Gamma_{A,\mu} = \sum_{\mu=1}^{2} (q_{A,\mu})^3 \mathit{\Gamma}_\mu \tag{2}$$

We now need a unitary which computes this function on a given state $|q_{A,\mu}\rangle |\Gamma_\mu\rangle |acc\rangle \to |q_{A,\mu}\rangle |\Gamma_\mu\rangle |acc + (q_{A,\mu})^3 \mathit{\Gamma}_\mu\rangle$. Consider having access to the following addition (multiplication) unitary $|A\rangle |B\rangle \to |A\rangle |A + (*)B\rangle$ as well as the unitary taking $|A\rangle \to |A^2\rangle$. We can now apply the following to get our desired unitary.

$$\begin{aligned}
&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y}\text{SQR}_x\text{MULT}_{x,y} |q_{A,\mu}\rangle_x |\Gamma_\mu\rangle_y |acc\rangle_z && (3)\\
=&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y}\text{SQR}_x |q_{A,\mu}\rangle_x |\Gamma_\mu q_{A,\mu}\rangle_y |acc\rangle_z && (4)\\
=&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y} |(q_{A,\mu})^2\rangle_x |\Gamma_\mu q_{A,\mu}\rangle_y |acc\rangle_z && (5)\\
=&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z} |(q_{A,\mu})^2\rangle_x |(q_{A,\mu})^3\Gamma_\mu\rangle_y |acc\rangle_z && (6)\\
=&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y} |(q_{A,\mu})^2\rangle_x |(q_{A,\mu})^3\Gamma_\mu\rangle_y |acc + (q_{A,\mu})^3\Gamma_\mu\rangle_z && (7)\\
=&\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x |(q_{A,\mu})^2\rangle_x |\Gamma_\mu q_{A,\mu}\rangle_y |acc + (q_{A,\mu})^3\Gamma_\mu\rangle_z && (8)\\
=&\text{MULT}^\dagger_{x,y} |q_{A,\mu}\rangle_x |\Gamma_\mu q_{A,\mu}\rangle_y |acc + (q_{A,\mu})^3\Gamma_\mu\rangle_z && (9)\\
=&|q_{A,\mu}\rangle_x |\Gamma_\mu\rangle_y |acc + (q_{A,\mu})^3\Gamma_\mu\rangle_z && (10)\\
& && (11)
\end{aligned}$$

This circuit to compute the inner sum in E^Γ could be called $E^\Gamma_{i\ (x,y,z)}$. Let us say we are given the following state

$$\bigotimes_A (|q_{A,1}\rangle_a |q_{A,2}\rangle_b) \otimes (|\Gamma_1\rangle_c |\Gamma_2\rangle_d |0\rangle_e)$$

we can now apply $\prod_a E^\Gamma_{i\ (a,c,e)} \prod_b E^\Gamma_{i\ (b,d,e)}$ to get

$$\bigotimes_A (|q_{A,1}\rangle_a |q_{A,2}\rangle_b) \otimes (|\Gamma_1\rangle_c |\Gamma_2\rangle_d |0\rangle_e) \to \bigotimes_A (|q_{A,1}\rangle_a |q_{A,2}\rangle_b) \otimes (|\Gamma_1\rangle_c |\Gamma_2\rangle_d |E^\Gamma\rangle_e)$$