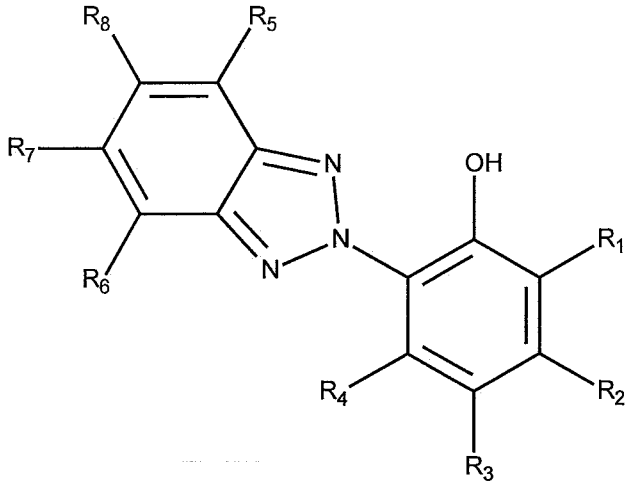
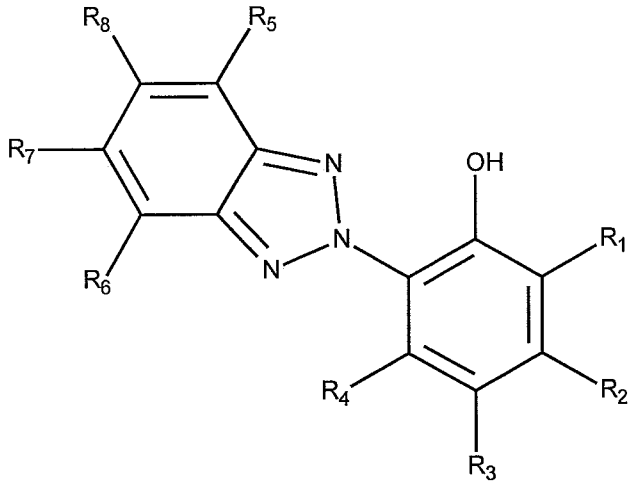
Among the embodiments disclosed herein are compositions comprising a substituted or unsubstituted benzotriazole phenol with the structure of Formula I:



Formula I

wherein if R^1 comprises a hydrogen atom; R^3 comprises an alkoxy or aryloxy group comprising 1-20 carbon atoms; and each R^2, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; or wherein if R^1 comprises an -O-R^9, a -N-R^9R^{10}, a -B(OR^{18})(OR^{19}) group, or a -SiR^{20}_3 group wherein R^9 comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, and R^{10} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, or R^9 and R^{10} together with the atoms connecting form a heterocyclic ring structure, each R^{18} and R^{19} is independently a hydrogen atom, an alkyl group, an aryl group, or R^{18} and R^{19} together with the atoms connecting form a heterocyclic ring structure, each R^{20} group is an alkyl group; and each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom.

In an aspect, there is provided a composition comprising a substituted benzotriazole phenol with the structure of Formula I:



Formula I

wherein if R^1 comprises a hydrogen atom; R^3 comprises an alkoxy or aryloxy group comprising 1-20 carbon atoms; and each R^2, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; or

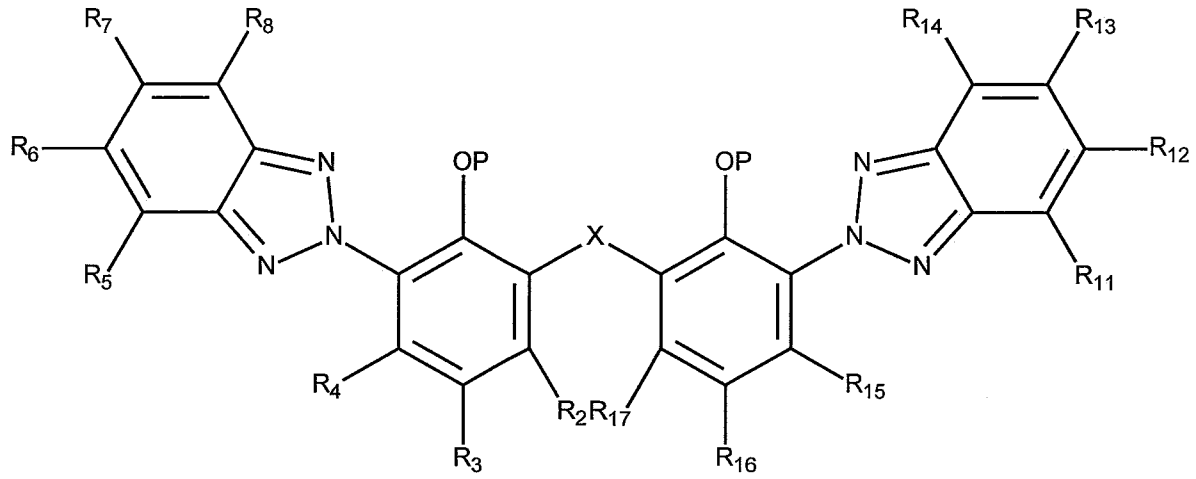
wherein if R^1 comprises an -O-R^9, a -N-R^9R^{10}, a -B(OR^{18})(OR^{19}) group, or a -SiR^{20}_3 group wherein R^9 comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, and R^{10} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, or R^9 and R^{10} together with the atoms connecting form a heterocyclic ring structure, each R^{18} and R^{19} is independently a hydrogen atom, an alkyl group, an aryl group, or R^{18} and R^{19} together with the atoms connecting form a heterocyclic ring structure, each R^{20} group is an alkyl group; and

each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom.

In some embodiments, the compositions comprise the structure of Formula II:

comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; or

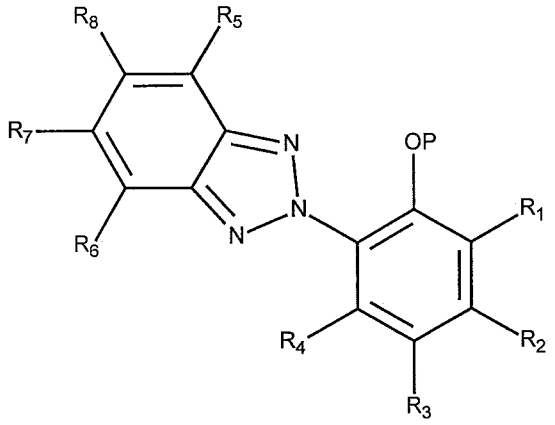
wherein if R^1 comprises an -O-R^9, a -N-R^9R^{10}, a -B(OR^{18})(OR^{19}) group, or a -SiR^{20}_3 group wherein R^9 comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, and R^{10} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, or R^9 and R^{10} together with the atoms connecting form a heterocyclic ring structure, each R^{18} and R^{19} is independently a hydrogen atom, an alkyl group, an aryl group, or R^{18} and R^{19} together with the atoms connecting form a heterocyclic ring structure, each R^{20} group is an alkyl group; and each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; or



Formula IV

wherein the group P is a protective group comprising an alkyl, a substituted alkyl, or a silyl group; and wherein X comprises an -O-, -NR^{10}-, -S(O)-, -$S(O)_2$-, or -S- linking group where R^{10} comprises a hydrogen atom, an alkyl group, or an aryl group, each R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^{11}, R^{12}, R^{13}, R^{14}, R^{15}, R^{16}, and R^{17}, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom.

In another aspect, there is provided a composition comprising a protected substituted benzotriazole phenol comprising the general structure Formula III or Formula IV:



Formula III

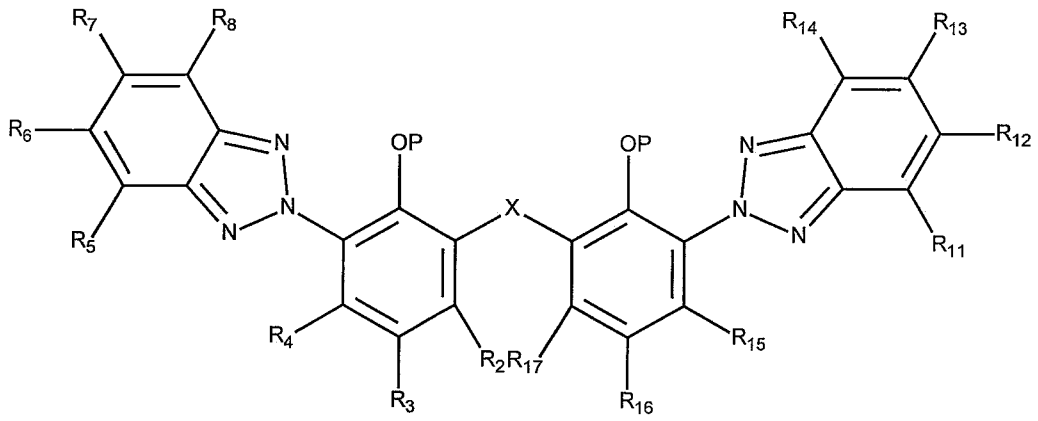
wherein the group P is a protective group comprising an alkyl, a substituted alkyl, or a silyl group;

and wherein if R^1 comprises a hydrogen atom; R^3 comprises an alkoxy or aryloxy group comprising 1-20 carbon atoms; and each R^2, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; or

wherein if R^1 comprises an -O-R^9, a -N-R^9R^{10}, a -B(OR^{18})(OR^{19}) group, or a –SiR^{20}_3 group wherein R^9 comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, and R^{10} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a heteroatom-containing group comprising one or more oxygen, nitrogen, sulfur, or phosphorous atoms, or R^9 and R^{10} together with the atoms connecting form a heterocyclic ring structure, each R^{18} and R^{19} is independently a hydrogen atom, an alkyl group, an aryl group, or R^{18} and R^{19} together with the atoms connecting form a heterocyclic ring structure, each R^{20} group is an alkyl group; and

each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom;

or



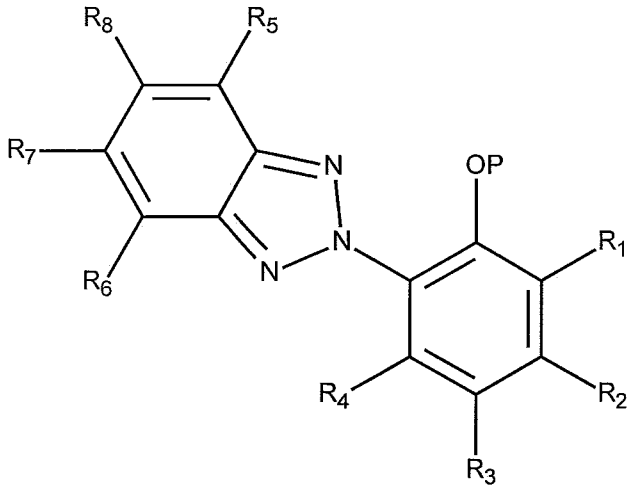
Formula IV

wherein the group P is a protective group comprising an alkyl, a substituted alkyl, or a silyl group;

and wherein X comprises an -O-, -NR^{10}-, -S(O)-, or -S- linking group where R^{10} comprises a hydrogen atom, an alkyl group, or an aryl group,

each R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^{11}, R^{12}, R^{13}, R^{14}, R^{15}, R^{16}, and R^{17}, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom.

Also disclosed herein are methods of preparing substituted benzotriazole phenols comprising providing a protected phenolic compound of Formula III:

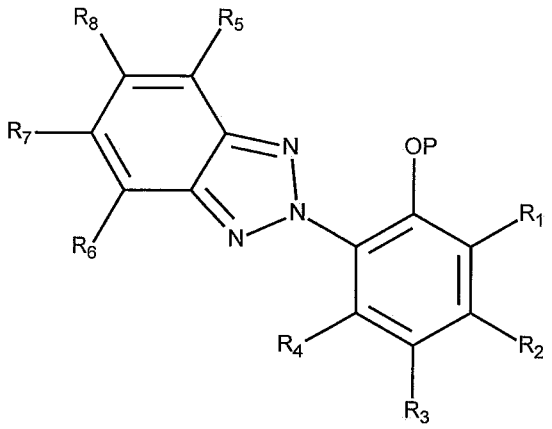


Formula III

wherein the group P is a protective group comprising an alkyl, a substituted alkyl, or a silyl group; R^1 comprises a leaving group selected from a halogen atom, a triflate group, a tosylate group, or a sulfonate group; and each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; providing a compound with the general formula R^{21}-Z-X-H wherein R^{21} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom; Z comprises an alkyl or aryl group, or a single bond; X comprises an -O-, -NR^{10}-, -S(O)-, -$S(O)_2$-, or -S- linking group where R^{10} comprises a hydrogen atom, an alkyl group, or an aryl group; providing a palladium-based catalyst comprising at least one palladium-phosphine complex; providing at least one base; providing at least one solvent; mixing the protected phenolic compound of Formula III, the compound with the general formula R^{21}-Z-X-H, the palladium-based catalyst, the at least one base, and the at least one solvent to form a reaction mixture; and heating the reaction mixture to a temperature of at least 100°C to effect a coupling reaction.

In another aspect, there is provided a method of preparing a substituted benzotriazole phenol comprising:

providing a protected phenolic compound of Formula III:



Formula III

wherein the group P is a protective group comprising an alkyl, a substituted alkyl, or a silyl group;

R^1 comprises a leaving group selected from a halogen atom, a triflate group, a tosylate group, or a sulfonate group; and

each R^2, R^3, R^4, R^5, R^6, R^7, and R^8, independently comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom;

providing a compound with the general formula R^{21}-Z-X-H wherein R^{21} comprises a hydrogen atom, an alkyl group, an alkenyl group, an aryl group, or a halogen atom;

Z comprises an alkyl or aryl group, or a single bond;

X comprises an -O-, -NR^{10}-, -S(O)-, or -S- linking group where R^{10} comprises a hydrogen atom, an alkyl group, or an aryl group;

providing a palladium-based catalyst comprising at least one palladium-phosphine complex;

providing at least one base;

providing at least one solvent;

mixing the protected phenolic compound of Formula III, the compound with the general formula R^{21}-Z-X-H, the palladium-based catalyst, the at least one base, and the at least one solvent to form a reaction mixture; and

heating the reaction mixture to a temperature of at least 100°C to effect a coupling reaction.

Detailed Description

One class of useful phenolics are 2-(2-hydroxyphenyl)benzotriazoles or benzotriazole phenols. Benzotriazole phenols are an important class of UV absorbers, and in some cases, can absorb in the visible range as well. These compounds are often used as additives in materials, particularly polymeric materials, and can be used as synthons to