Supporting Information

HIGH EFFICIENCY RADICAL PHOTOPOLYMERIZATION ENHANCED BY AUTONOMOUS DARK CURE

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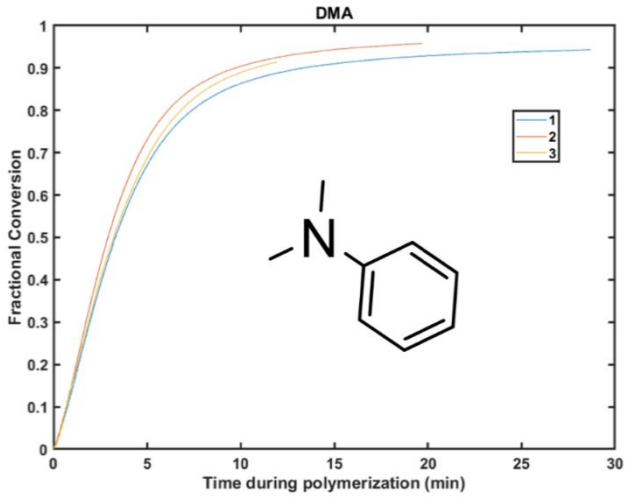


Figure S1. Redox polymerization profiles of *N,N*-dimethylaniline (DMA) for **Figure 2**. The experimental conditions include 3 mol% concentrations of both DMA and BPO in di(ethylene glycol) ethyl ether acrylate.

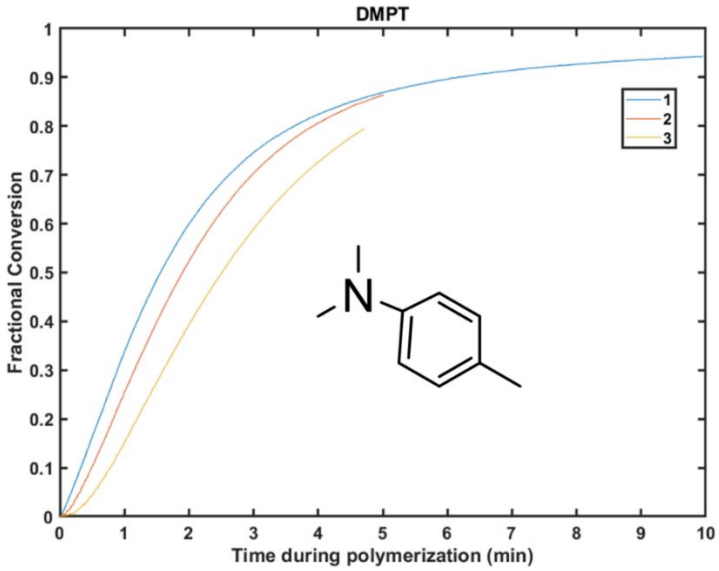


Figure S2. Redox polymerization profiles of N,N-dimethyl-p-toluidine (DMPT) for **Figure 2**. The experimental conditions include 3 mol% concentrations of both DMA and BPO in di(ethylene glycol) ethyl ether acrylate.

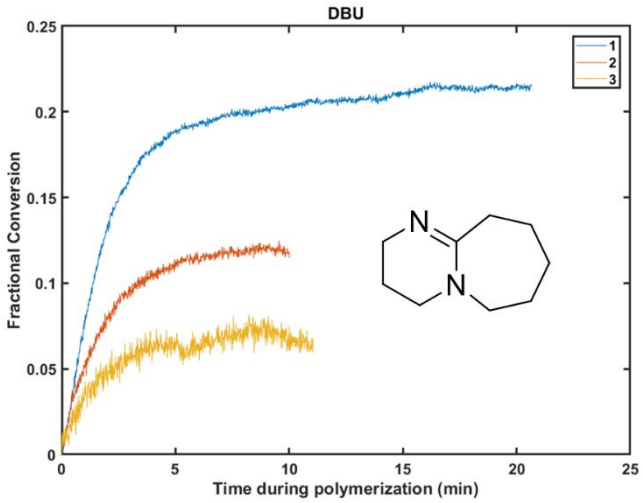


Figure S3. Redox polymerization profiles of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) for **Figure 2**. The experimental conditions include 3 mol% concentrations of both DMA and BPO in di(ethylene glycol) ethyl ether acrylate.

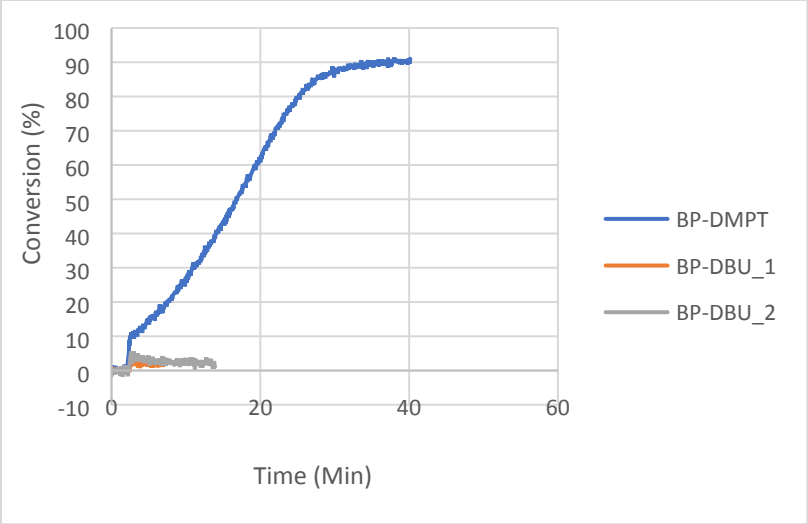


Figure S4. Polymerization profiles of two DCPIs that release DMPT (BP-DMPT) and DBU (BP-DBU), respectively. The resin composition is 90% TEGDMA and 10% acrylonitrile with 2 mol% BPO and 1 mol% respective photoinitiators. As acetonitrile is susceptible to Michael addition, more nucleophilic DBU attacks acetonitrile and limits the radical-mediated chain growth polymerization while non-nucleophilic DMPT avoids such side reactions and proceeds to react with BPO to induce dark-curing.

SI. Thin Film Approximation

According to Beer-Lambert, $A = \varepsilon c l$ where ε is molar absorptivity, c is molar concentration of photochemical species, l is path length.

The UV-Vis spectra (**Figure S11** and **S13**) indicate that DCPI and CTPI absorb light with a similar absorptivity ($\varepsilon = 80.1\ L/cm/mol$). The molar concentration (c) in our experiments was 0.007 mol/L while the path length (l) of the samples were 0.11 cm.

Hence, $A = 80.1\ X\ 0.007\ X\ 0.11 = 0.062$

Reorganizing $A = -logT$ yields $10^{-A} = T$

Plugging in A value, $T = 10^{-0.062} = 0.87$.

Therefore, the minimal irradiance gradient introduced across the sample pathlength here effectively validates the optically thin film approximation.

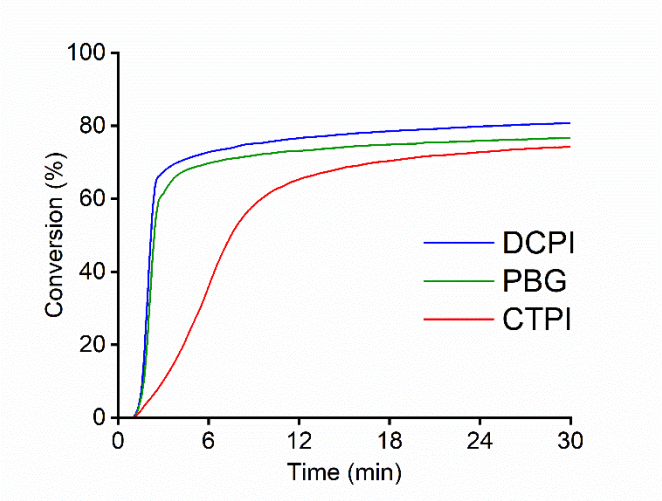


Figure S5. Photopolymerization kinetic profiles of DCPI, PBG, and CTPI under full cure. DCPI and PBG have similar kinetics while CTPI is slower. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP] = [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [DMPT] = [BPO] = 23.1 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

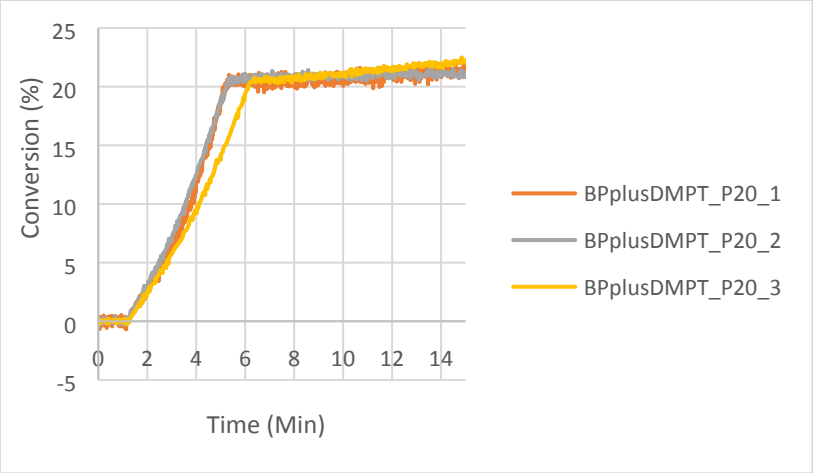


Figure S6. Partial cure polymerization profiles of CTPI composed of BP sensitizer and DMPT co-initiator. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP] = 7.7 µmol/g of resin and [DMPT] = 23.1 µmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

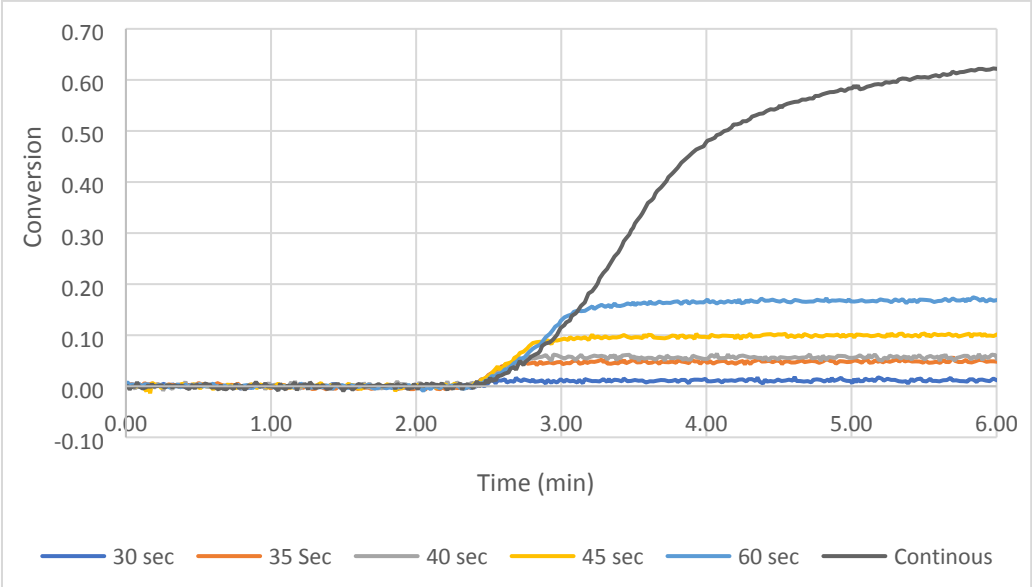


Figure S7. Polymerization profiles of DMPA (2,2-dimethoxy-2-phenylacetophenone) with varying irradiation durations. The conditions of these polymerizations included illumination with a 10 mW/cm^2 320-390 nm filter arc lamp with [DMPA] = 0.025 mol% in TEGDMA.

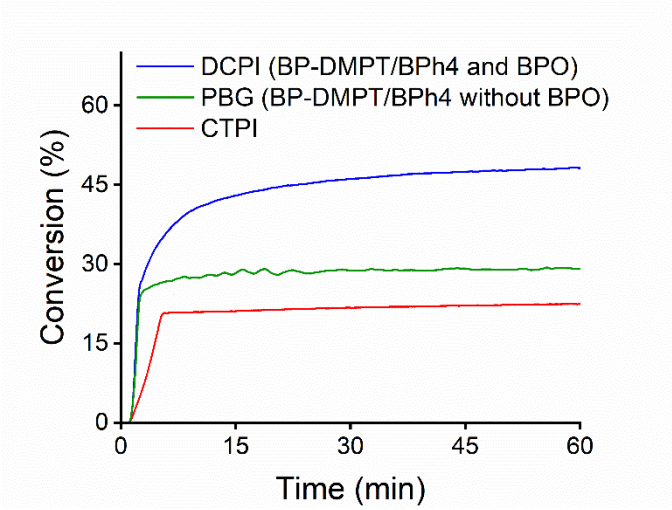


Figure S8. Photopolymerization kinetic profiles of DCPI, PBG, and CTPI under 20% partial cure. DCPI shows dark-curing while PBG and CTPI does not. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP] = [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [DMPT] = [BPO] = 23.1 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

SI. Kinetic Property Calculations

Based on a steady-state analysis, the rate of methacrylate free radical polymerization (R_p) can be expressed as[1]

$$\frac{k_p}{k_t^{1/2}} = \frac{R_p}{[M](\varepsilon I_0 \Phi[I])^{1/2}} \qquad \textbf{Eq. 1}$$

Whereas k_p is propagation kinetic constant, k_t is termination kinetic constant. The molar concentration of monomer is represented by [M], the initiator molar absorption by ε, light intensity by I_0, initiator efficiency by Φ, and the initiator concentration by [I]. Therefore, the initiator efficiency can be calculated by reorganizing **Eq. 1**

$$\boldsymbol{\Phi} = \frac{\boldsymbol{k_t R_p^2}}{\boldsymbol{\varepsilon I_0 [I]([M]k_p)^2}} \qquad \textbf{Eq 2}$$

Based on **Figure S5**, R_p for each system was calculated based on the time that it took the reaction proceed from 10% to 20% conversion. $\frac{\boldsymbol{k_p}}{\boldsymbol{k_t^{1/2}}}$ for TEGDMA was obtained from the previous literature, where $\boldsymbol{k_p}$ is 516 $\mathrm{M^{-1}s^{-1}}$ and k_t is 5 x 10^5 $\mathrm{M^{-1}s^{-1}}$.[1] From **Figure S11**, the molar absorptions for BP, PBG, and DCPI at 365nm are nearly identical (ε= 0.8 L/m/mol). Initiator concentration [I] is 0.007mol/L. Light intensity I_0 is 300 W/m^2

Hence, $\boldsymbol{\Phi}$ for DCPI can be determined as

$$\boldsymbol{\Phi} = \frac{\boldsymbol{k_t R_p^2}}{\boldsymbol{\varepsilon I_0 [I]([M]k_p)^2}} = \frac{\boldsymbol{5 * 10^5 * 4.5^2}}{\boldsymbol{0.8 * 300 * 0.007 * (5.5 * 516)^2}} \textbf{=0.75}$$

Similar calculations were done with PBG and CTPI.

Table S1. Rate of polymerization and initiator efficiency of photoinitiators

	CTPI	PBG	DCPI
R_p ($\mathrm{M^{-1}s^{-1}}$)	0.68	3.40	4.50
Φ	0.02	0.43	0.75

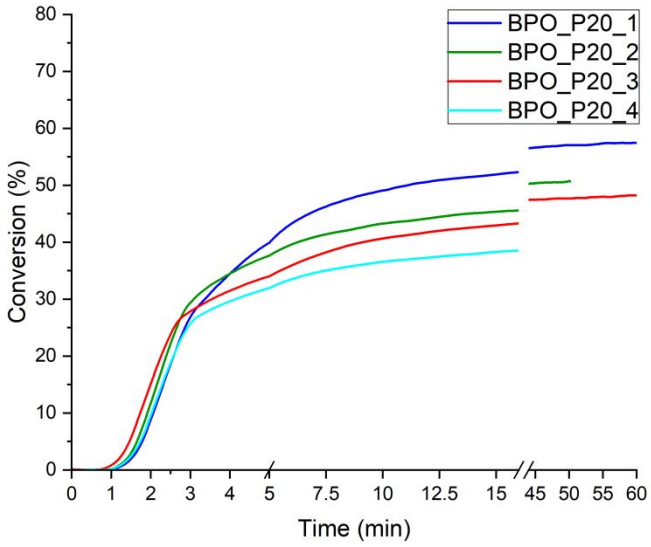


Figure S9. Polymerization profiles of DCPI under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [BPO] = 23.1 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

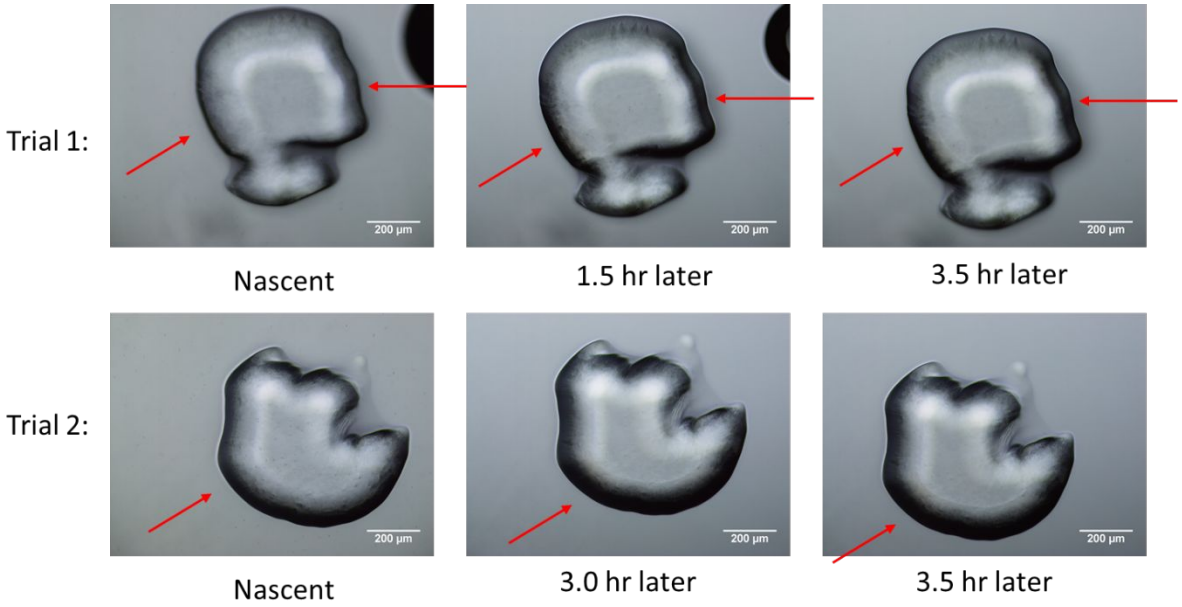
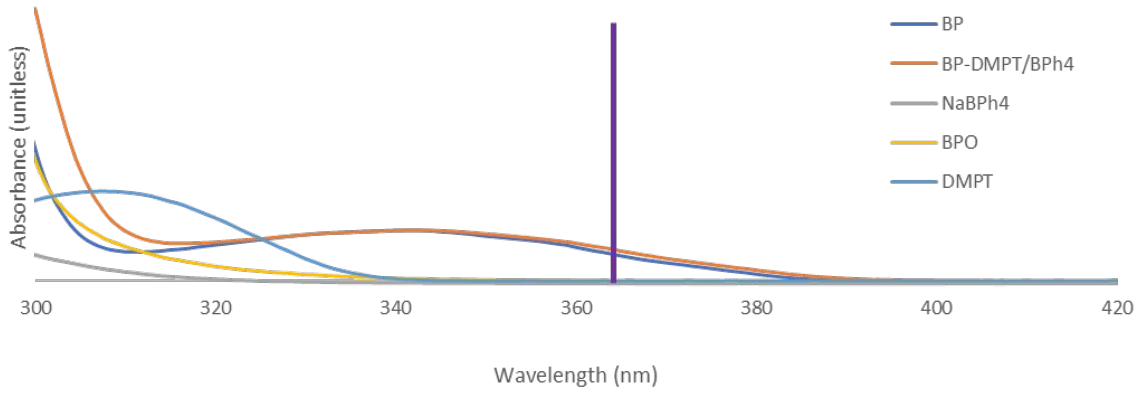


Figure S10. Visual development of dark-cured polymer using a microscope. As polymerization proceeds further by dark-curing and the refractive index of polymer changes, the edges of a pin-hole polymer become darker.

A



B

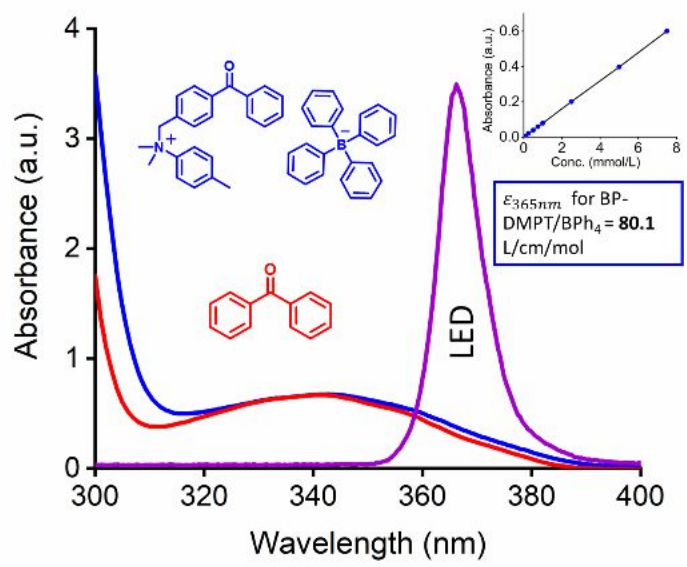


Figure S11 A and B. UV-Vis spectra of initiating components of DCPI and CTPI in dimethylformamide (DMF). The concentrations are 0.5 mM DMPT, 5 mM BP, 5 mM BP-DMPT/BPh_4, 50 mM $NaBPh_4$, and 50mM BPO. BP-DMPT/BPh4 and BP essentially have the same molar absorptivity at 365 nm while other components do not absorb at 365 nm. The Inset shows concentration-dependent absorbance of BP-DMPT/BPh4 at 365 nm, resulting in molar absorption coefficient (ε) = 80.1 L/cm/mol at 365 nm. the photophysical properties of these photoinitiators based on benzophenone chromophore do not significantly differ in regards to intersystem crossing efficiency, excited state energies, or absorbance.[2–4]

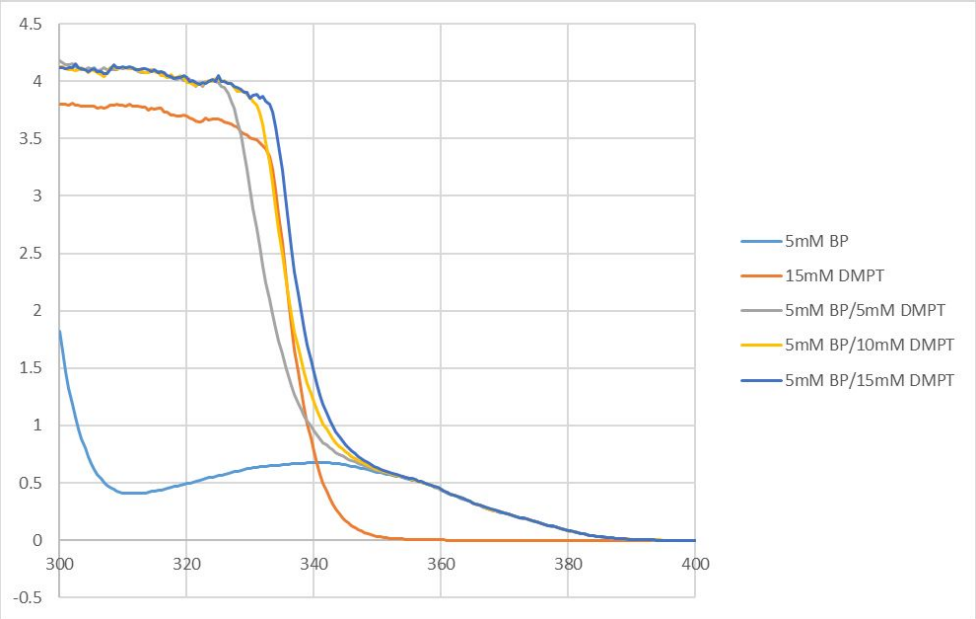


Figure S12. UV-Vis Spectra of BP with varying concentrations of DMPT. When BP and DMPT are added, a new spectrum is identical to the two spectra of BP and DMPT added to each other, which means a lack of ground state interaction (e.g. charge transfer complex) between BP and DMPT.

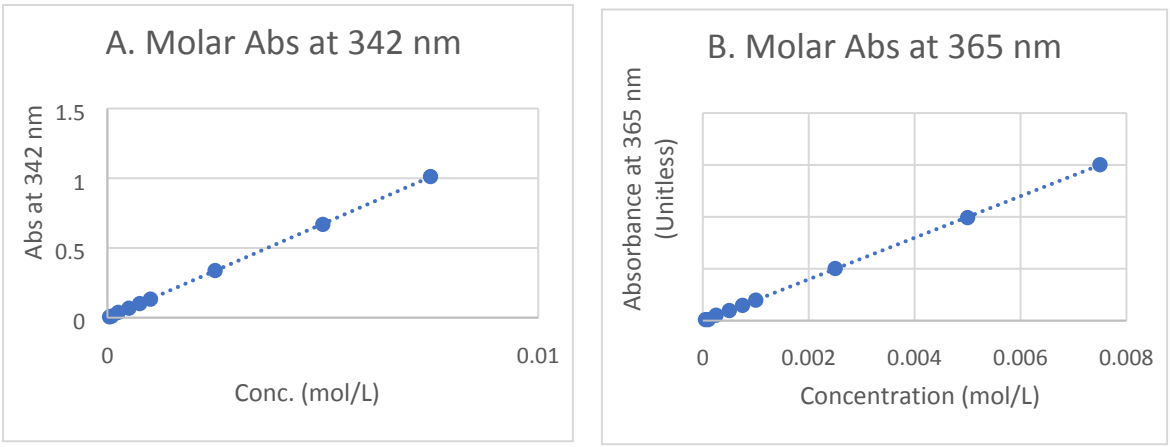


Figure S13 A and B. Molar Absorptivity of BP-DMPT/BPh4 in DMF at lambda max of 342 nm and irradiation wavelength of 365 nm.

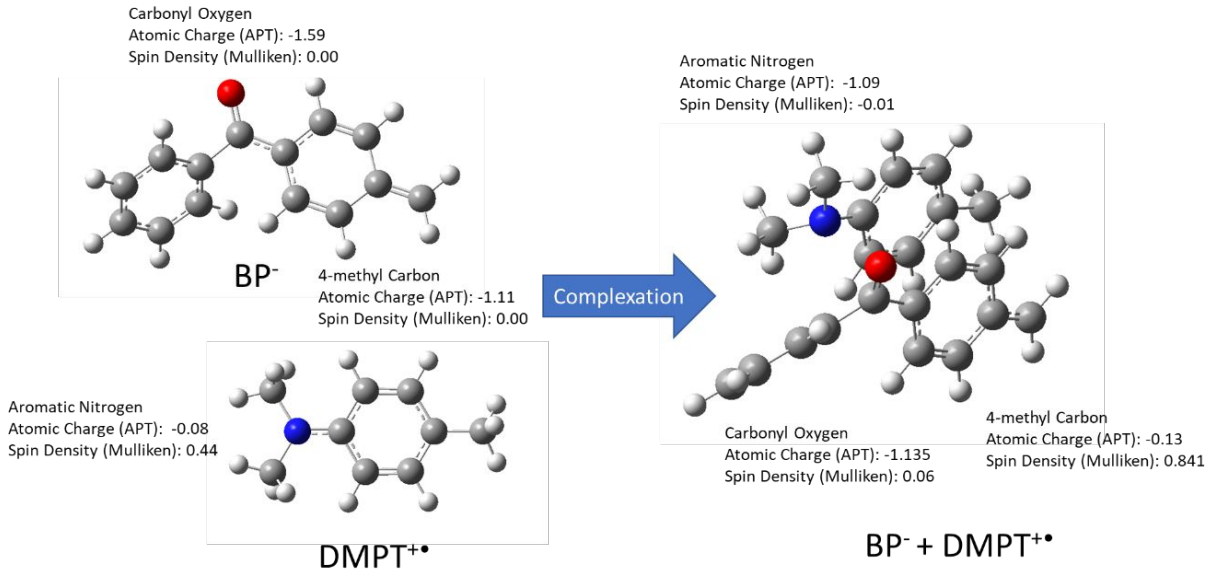


Figure S14. Charge-transfer complex formation between BP^- and $DMPT^{+\bullet}$. Anionic charges of BP^- were transferred to $DMPT^{+\bullet}$ while spin density of $DMPT^{+\bullet}$ was transferred to BP^-.

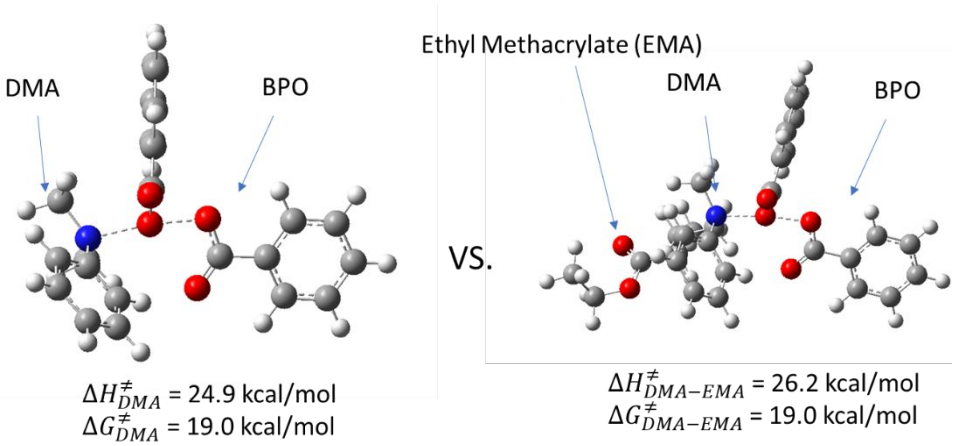


Figure S15. Transition states of DMA attacking BPO and DMA tethered to methacrylate attacking BPO. Activation barrier difference between these two initiators are marginal. See reference 5 (Kangmin Kim, 2019, JACS) for the detailed nature of the transition state.[5]

Details of Quantitative NMR for **Figure 6**.

In order to account for the amine photogeneration in our system, three sets of hydrogens can be tracked via H-NMR. Hydrogens at para-methyl group of DMPT are a singlet with an integration of 3 at 2.22 ppm (DMPT-p-methyl-H). Hydrogens at N,N-dimethyl group of DMPT are a singlet with a integration of 6 at 2.85 ppm. (DMPT-N,N-dimethyl-H) Hydrogens in the aromatic regions of DMPT are doublet with a integration of 2 at 6.68 ppm and another integration of 2 at 7.02 ppm. Using aromatic hydrogens would be intractable due to the presence of numerous aromatic hydrogens in vicinity from BP moiety and BPh4 counterion. Also, we soon realized that DMPT-p-methyl-H overlaps with the methyl hydrogen of the photolyzed BP-moiety from BP-DMPT.

Therefore, we decided to track the appearance of DMPT-N,N-dimethyl-H signal to quantify the amine photogeneration. We also tracked the disappearance of the analogous peak signals (BP-DMPT-N,N-dimethyl-H) from the caged amine species in the PBG in order to confirm that the appearance of DMPT and disappearance of PBG are making up 100% of DMPT in either form. If we found that 100% of DMPT are present, then it can indicate that the undesired side reactions that may destroy the amine are minimal. Such reactions may be imine formation by losing a N-methyl group. For the reference peak to use as a constant integration, we initially tried to use aromatic signals but their integration was found to be unreliable due to a short recycle delay that prevent the nuclei relaxation after a pulse. Instead, we chose to use ethylene carbonate peak for the internal standard.

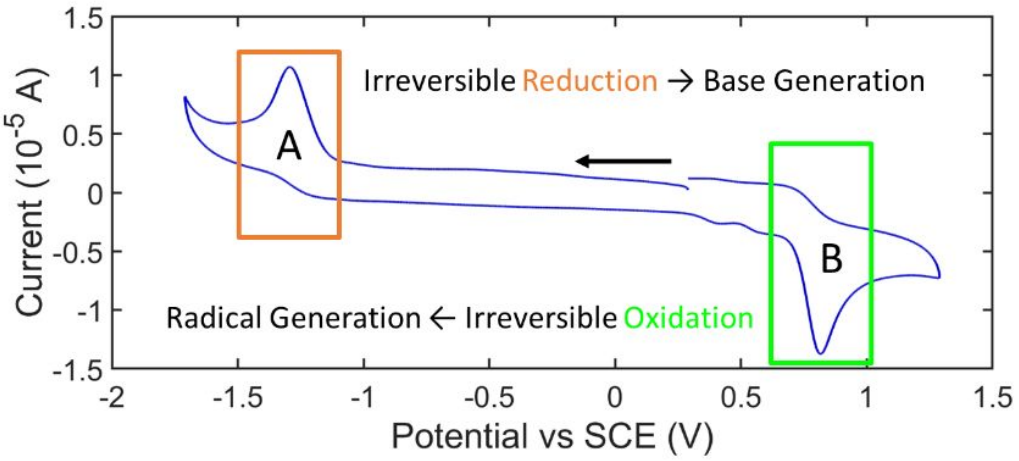


Figure S16. Cyclic voltammogram of BP-DMPT/BPh_4. Both reduction of BP-DMPT and oxidation of BPh_4 are irreversible under our experimental conditions, which contributes to efficient photopolymerization and dark curing. The initial scan direction was negative, as indicated by the arrow, and CVs were collected in room temperature acetonitrile under Ar with a 0.01 M

$Ag/AgNO_3$ electrode and 0.1 M tetrabutylammonium hexafluorophosphate, and scanned at a rate of 100 mV/s.

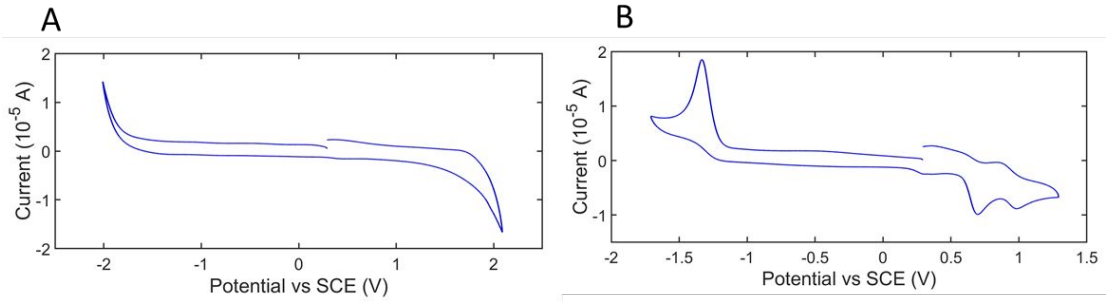


Figure S17.A. Cyclic voltammogram of acetonitrile at room temperature under argon atmosphere, taken at a scan rate of 100 mV/s. The initial scan direction was negative. Acetonitrile provides a sufficiently wide range of voltage for our experiments. **B.** Cyclic voltammogram of BP-DMPT/Br in room temperature acetonitrile under argon atmosphere, taken at a scan rate of 100 mV/s. The initial scan direction was negative. The reduction peak corresponds to the reduction of BP-DMPT, similar to what was discussed in the manuscript. However different oxidation behaviors were observed regarding bromide counter ion.

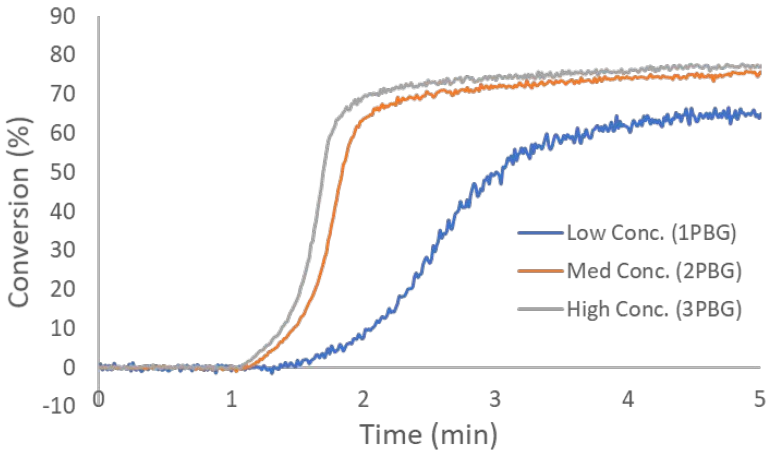


Figure S18. Photopolymerization profiles of photo-base-generator (PBG, BP-DMPT/BPh4) with its various concentrations under full irradiation conditions. Low (1PBG), Med (2PBG), and High (3PBG) corresponds to [BP-DMPT/BPh4] = 7.7; 15.4; and 23.1 μmol/g of resin with 90 wt% TEGDMA and 10 wt% MBL composition. With higher concentrations of PBG, polymerization rates are too rapid which limited our ability to reliably shutter the illumination at desired intervals. The experimental conditions include 30mW/cm2 365nm LED.

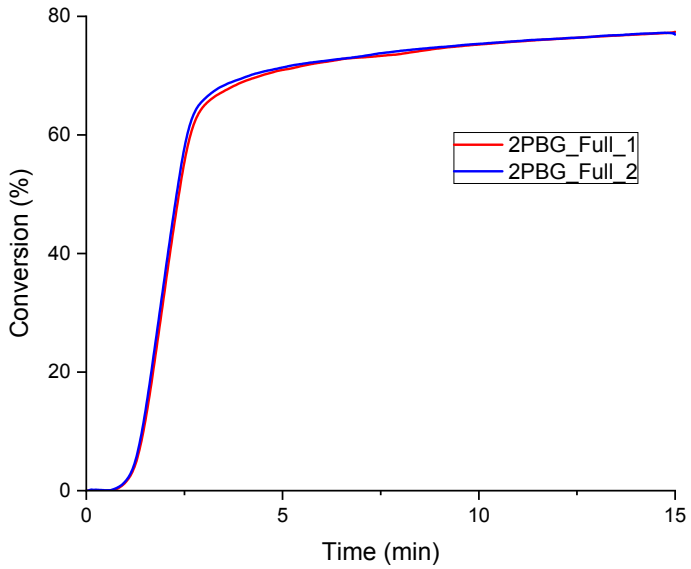


Figure S19. Photopolymerization profiles of medium concentration photo-base-generator (PBG, BP-DMPT/BPh4) under full irradiation conditions. medium (2PBG) corresponds to [BP-DMPT/BPh4] = 15.4 μmol/g of resin with 90 wt% TEGDMA and 10 wt% MBL composition. The experimental conditions include 30mW/cm2 365nm LED.

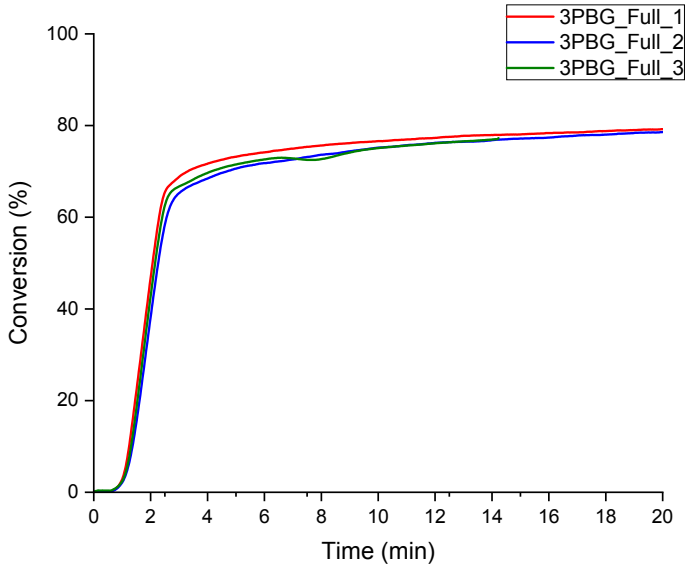


Figure S20. Photopolymerization profiles of high concentration photo-base-generator (PBG, BP-DMPT/BPh4) under full irradiation conditions. High (3PBG) corresponds to [BP-DMPT/BPh4] = 23.1 μmol/g of resin with 90 wt% TEGDMA and 10 wt% MBL composition. The experimental conditions include 30mW/cm2 365nm LED.

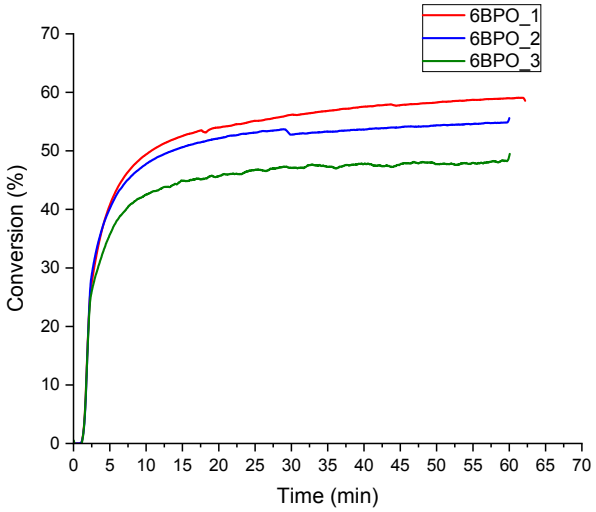


Figure S21. Polymerization profiles of DCPI with medium concentration of BPO under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and 6BPO = [BPO] = 46.2 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

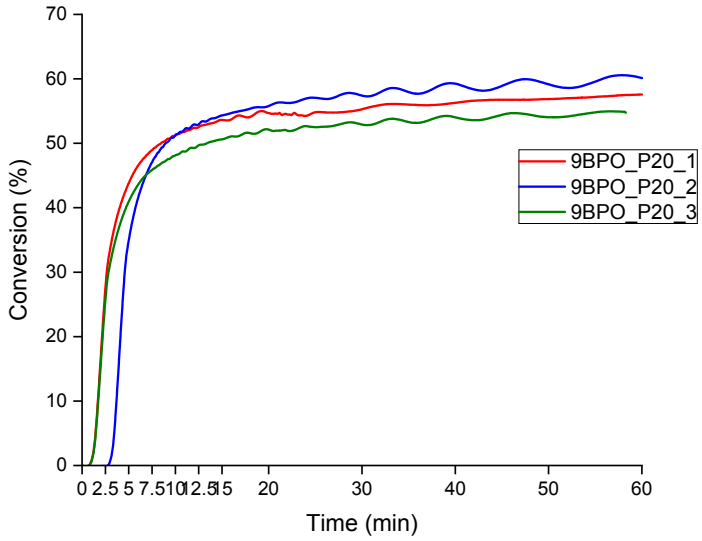


Figure S22. Polymerization profiles of DCPI with high concentration of BPO under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and 9BPO = [BPO] = 69.3 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

Details of Resin Design for **Figure 8.B**

We refrained from introducing any confounding components that may change coordination (e.g. hydrogen bonding), ensuring that, between samples, no drastic initial viscosity differences were observed as well as minimizing the influence of such coordination changes on polymerization

kinetics.[6] Additionally, because larger monomers/oligomers can induce unexpected changes in polymerization behavior, we maintained an approximately constant reactive group density by combining n-butyl methacrylate (BMA) with triethylene glycol dimethacrylate (TEGDMA) because BMA has approximately half the molecular weight of the di-vinyl TEGDMA.

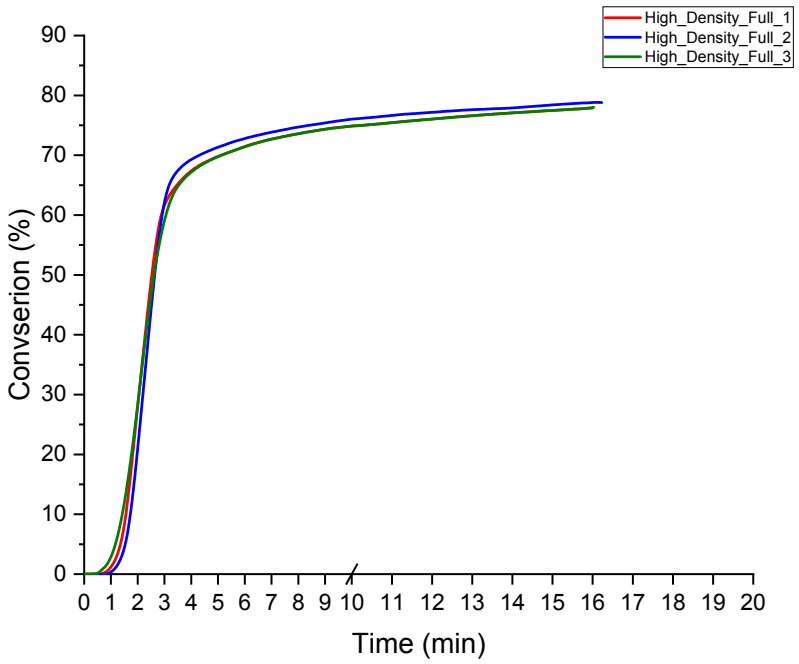


Figure S23. Polymerization profiles of DCPI in HiCxLR under full cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 µmol/g of resin and [BPO] = 46.2 µmol/g of resin.

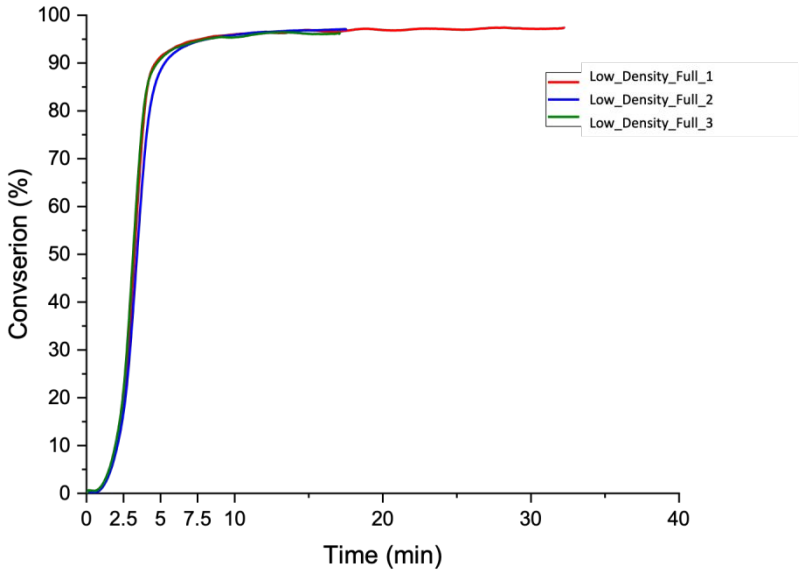


Figure S24. Photopolymerization profile of LoCxLR under full irradiation condition. LoCxLR is composed of 50wt% TEGDMA, 10wt% MBL, and 40 wt% BMA. The experimental conditions include 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [BPO] = 46.2 μmol or 1.12 wt%/g of resin.

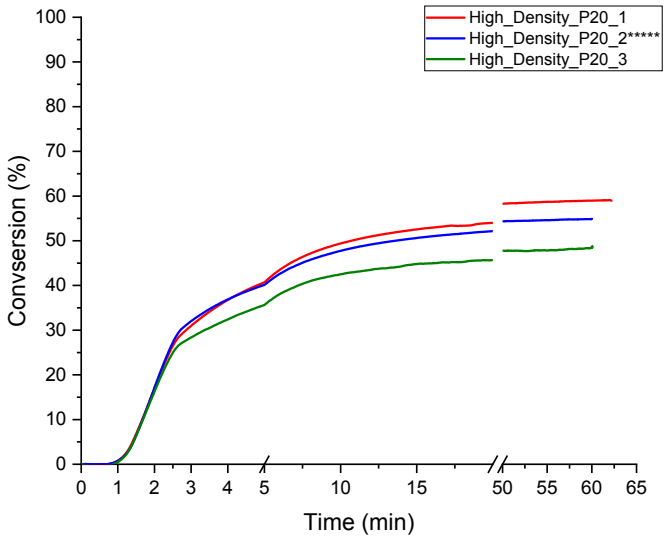


Figure S25. Polymerization profiles of DCPI with low concentration of BPO under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [BPO] = 46.2 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

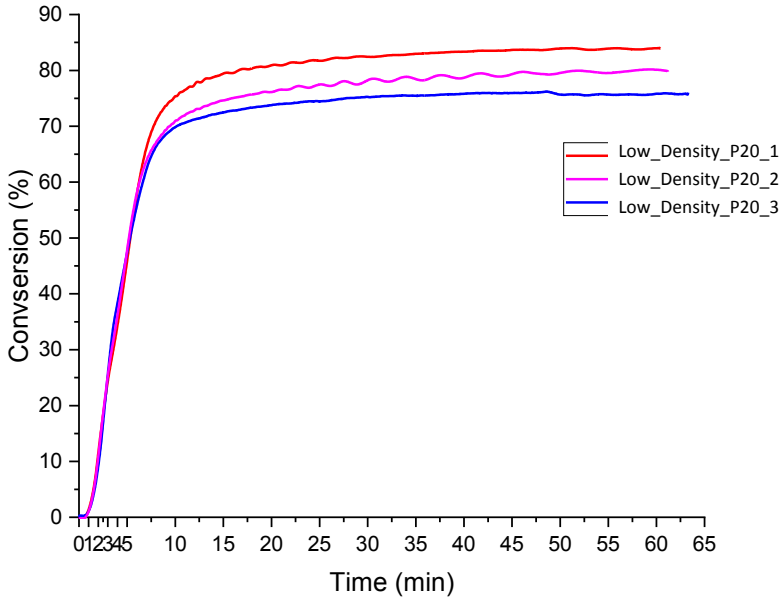


Figure S26. Polymerization profiles of DCPI in LoCxLR under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 30 mW/cm^2 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and [BPO] = 46.2 μmol/g of resin.

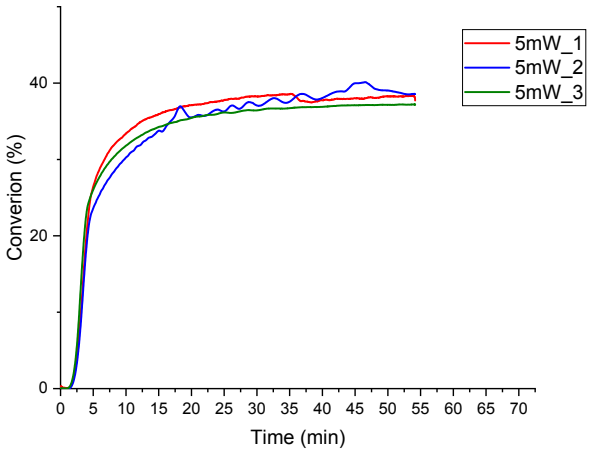


Figure S27. Polymerization profiles of DCPI with 5 mW/cm^2 under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 365 nm LED with [BP-DMPT/BPh4] = 7.7 μmol/g of resin and 6BPO = [BPO] = 46.2 μmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

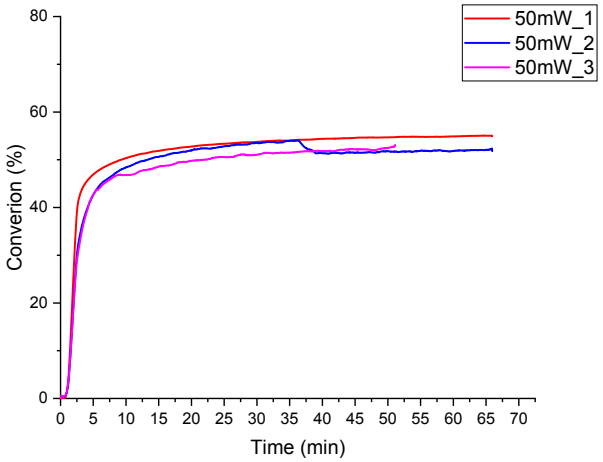


Figure S28. Polymerization profiles of DCPI with 50 mW/cm^2 under 20% partial cure regimes. The conditions of these polymerizations included illumination with a 365 nm LED with [BP-

DMPT/BPh4] = 7.7 µmol/g of resin and 6BPO = [BPO] = 46.2 µmol/g of resin in HiCxLR with a TEGDMA/MBL (9:1 mass fraction) composition.

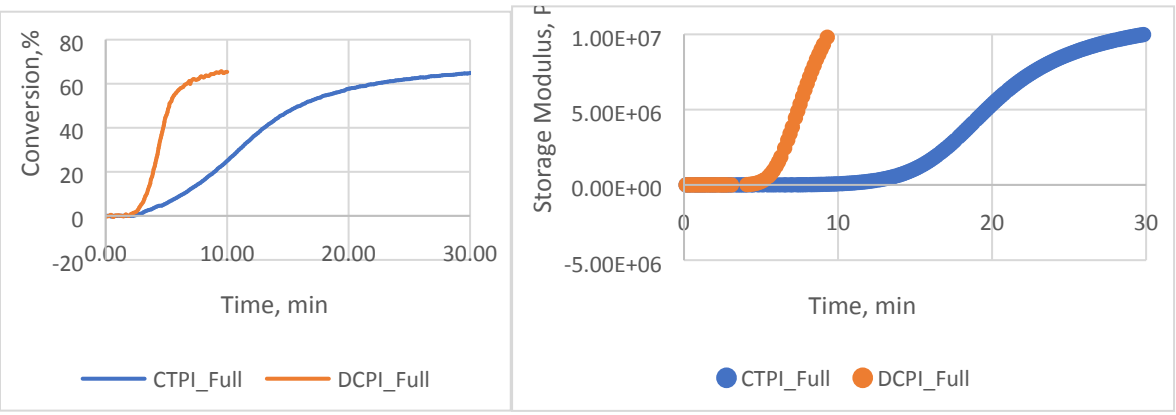


Figure S29. Polymerization profile and corresponding storage modulus development of CTPI and DCPI under full cure protocol, using a photo-rheometer coupled with FT-IR. Despite different photopolymerization rates, CTPI and DCPI reached similar storage modulus at vitrification, as expected.The experimental conditions include a 365 nm-filtered Hg arc lamp with [BP-DMPT/BPh4] = 7.7 µmol/g and [BPO] = 23.1 µmol/g of HiCxLR resin at ambient temperature. The rotational rheometer was used with 0.5% strain and 1 Hz oscillation frequency while intensities of 4.4 mW/cm^2 was used.

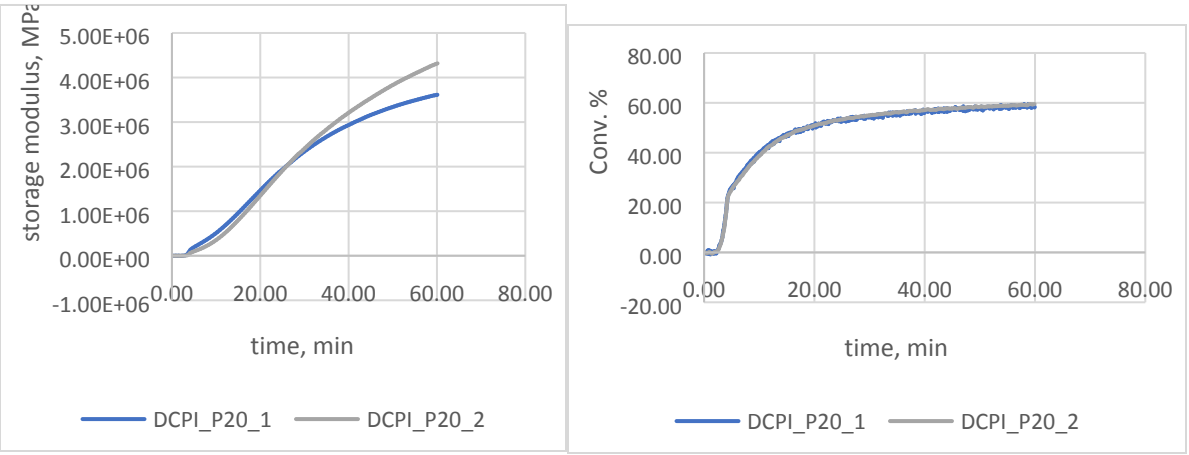


Figure S30. Polymerization profile and corresponding storage modulus development of DCPI under 20% partial cure protocol, using a photo-rheometer coupled with FT-IR. The experimental conditions include a 365 nm-filtered Hg arc lamp with [BP-DMPT/BPh4] = 7.7 μmol/g and [BPO] = 23.1 μmol/g of HiCxLR resin at ambient temperature. The rotational rheometer was used with 0.5% strain and 1 Hz oscillation frequency while intensities of 4.4 mW/cm^2 was used.

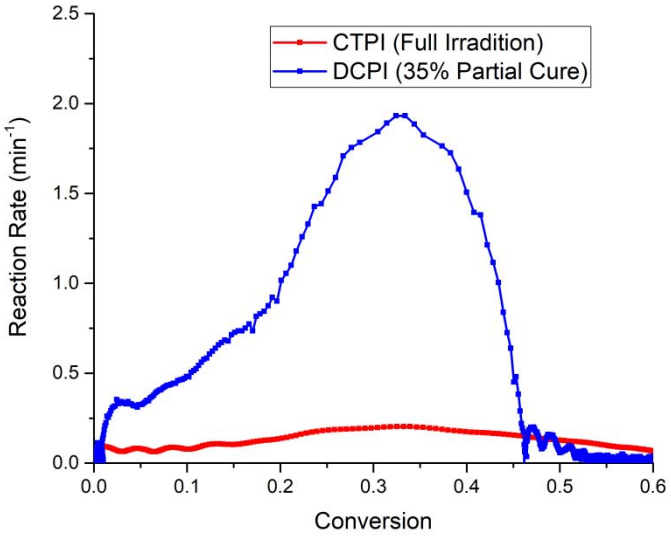


Figure S31. Polymerization rate changes with respect to conversion in experiments for Figure 9.B. Initially, a higher photopolymerization rate of DCPI results in higher stress, relative to that of CTPI. However, at ~45% conversion, CTPI has a higher photopolymerization than a dark-curing rate of DCPI. As a result, CTPI's stress surpasses DCPI's.

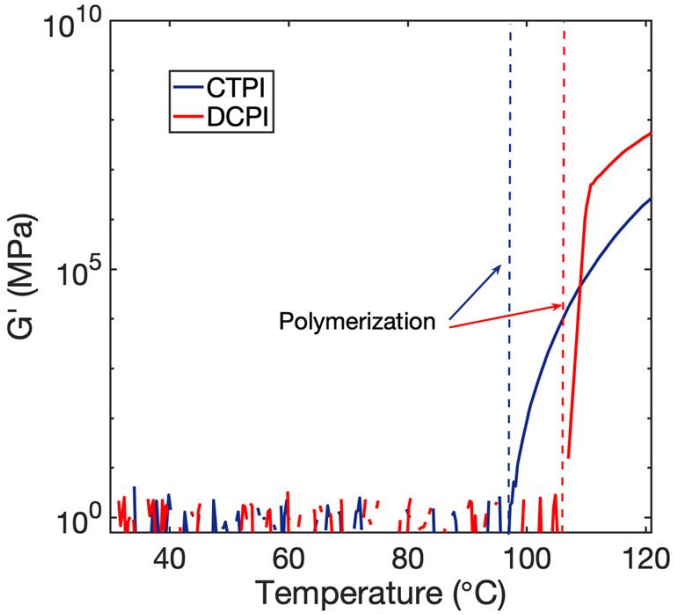


Figure S32. Thermal response of CTPI and DCPI resins measured by rheometer. Both resins started to polymerize around 100 ºC.

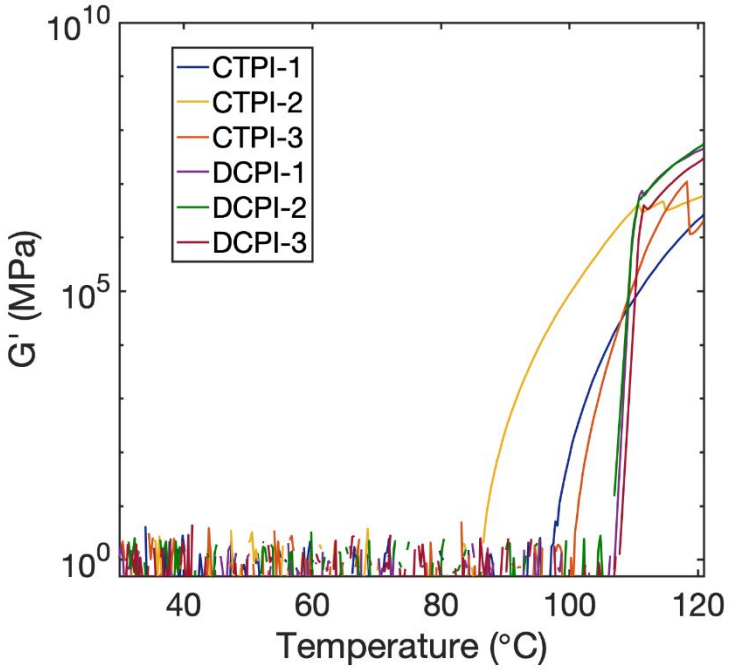


Figure S33. Thermal response of CTPI and DCPI resins measured by rheometer. Both resins started to polymerize at approximately 100 ºC.

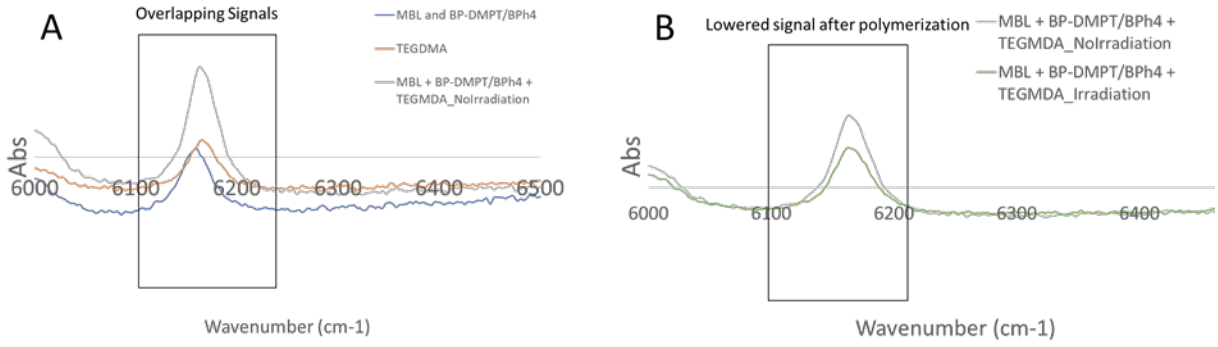


Figure S34.A. IR spectra of MBL and TEGDMA. **B.** lowered IR signal after polymerization.

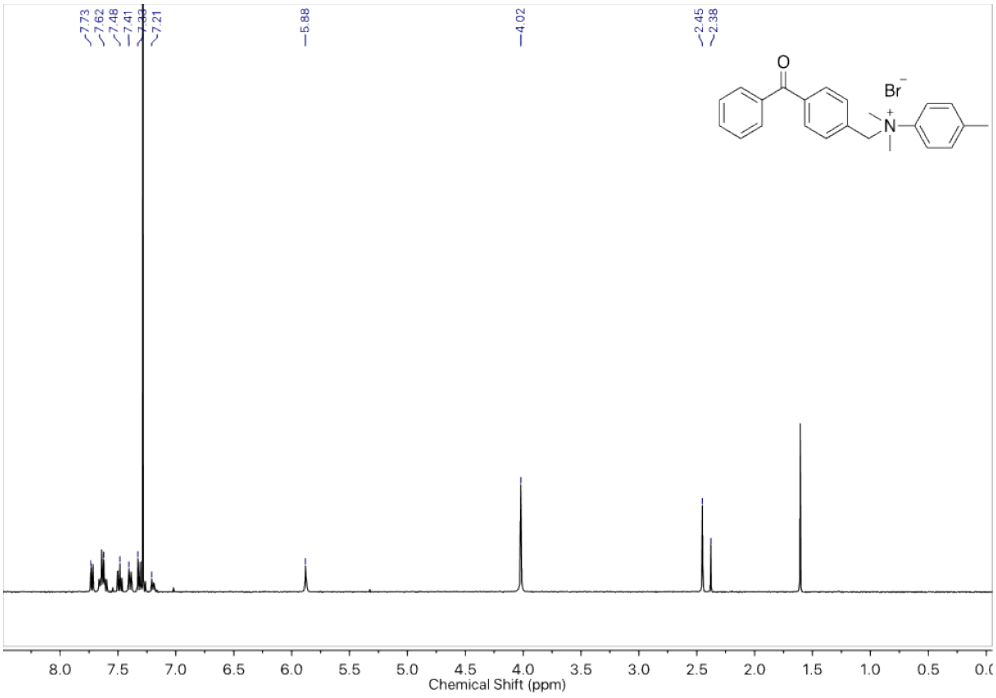


Figure S35. ^{1}H-NMR of BP-DMPT/Br

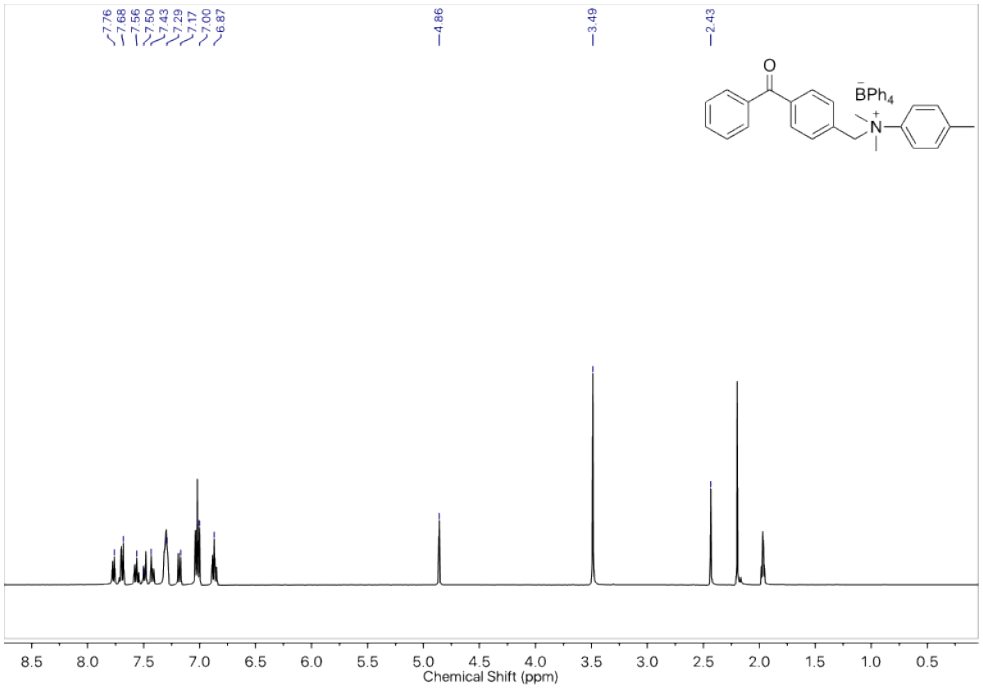


Figure S36. ^{1}H-NMR of BP-DMPT/BPh_4

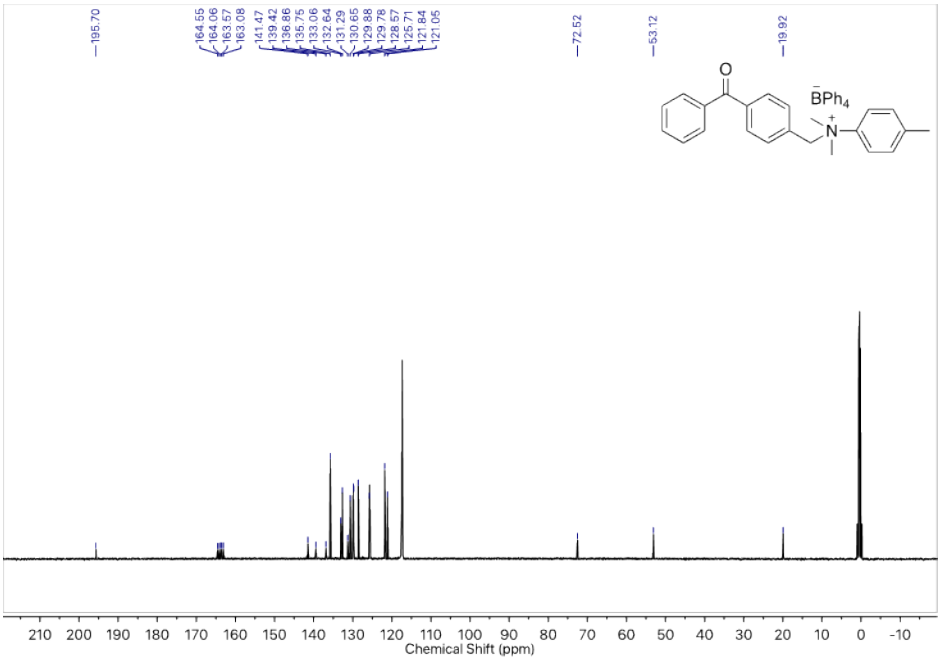


Figure S37. ^{13}C-NMR of BP-DMPT/BPh_4

References

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Atomic Coordinates of Chemical Species

BP-DMPT Ground State

ZPE = -1019.93

N	4.3791	-0.2846	0.2716
C	4.0179	-0.8328	1.6249
H	3.0764	-0.3812	1.9354
H	3.9124	-1.9144	1.5669
H	4.8170	-0.5643	2.3157
C	4.3654	1.2089	0.3850
H	4.5320	1.6484	-0.5979
H	3.3905	1.5065	0.7665
H	5.1442	1.5079	1.0860
C	3.3652	-0.7349	-0.7899
H	3.7658	-0.3670	-1.7366
H	3.3959	-1.8253	-0.7846
C	1.9618	-0.2418	-0.5645
C	1.5360	0.9537	-1.1549
C	1.0556	-0.9935	0.1897
C	0.2364	1.4073	-0.9663
H	2.2255	1.5296	-1.7660

C	-0.2557	-0.5551	0.3599
H	1.3722	-1.9314	0.6391
C	-0.6683	0.6514	-0.2139
H	-0.0914	2.3421	-1.4105
H	-0.9496	-1.1465	0.9498
C	-2.0484	1.2044	-0.0014
C	-3.2204	0.2793	0.0523
C	-3.2295	-0.9447	-0.6274
C	-4.3594	0.6928	0.7549
C	-4.3700	-1.7455	-0.6039
H	-2.3600	-1.2618	-1.1955
C	-5.4886	-0.1180	0.7932
H	-4.3446	1.6493	1.2683
C	-5.4951	-1.3372	0.1117
H	-4.3802	-2.6860	-1.1457
H	-6.3655	0.1998	1.3487
H	-6.3799	-1.9663	0.1350
O	-2.1973	2.4091	0.1230
C	5.7189	-0.8039	-0.1480

C	6.7332	0.0559	-0.5513
C	5.9228	-2.1852	-0.1572
C	7.9604	-0.4766	-0.9525
H	6.6079	1.1307	-0.5631
C	7.1503	-2.6947	-0.5596
H	5.1410	-2.8753	0.1402
C	8.1929	-1.8510	-0.9643
H	8.7483	0.2046	-1.2606
H	7.3005	-3.7709	-0.5588
C	9.5113	-2.4234	-1.4090
H	9.3962	-2.9630	-2.3548
H	10.2551	-1.6370	-1.5540
H	9.8965	-3.1336	-0.6714

Tetraphenyl Borate

ZPE = -950.88

B	0.0000	0.0026	0.0020
C	-0.0172	1.5080	-0.6721

C	-0.8754	2.4955	-0.1441
C	0.7659	1.9094	-1.7665
C	-0.9394	3.7915	-0.6530
H	-1.5206	2.2332	0.6946
C	0.7119	3.2047	-2.2961
H	1.4369	1.1917	-2.2336
C	-0.1392	4.1564	-1.7397
H	-1.6162	4.5172	-0.2077
H	1.3349	3.4652	-3.1488
H	-0.1856	5.1630	-2.1466
C	0.8700	-1.0468	-0.9276
C	2.2741	-0.9237	-0.9856
C	0.3231	-2.0970	-1.6827
C	3.0759	-1.7696	-1.7502
H	2.7548	-0.1374	-0.4033
C	1.1117	-2.9605	-2.4533
H	-0.7524	-2.2598	-1.6683
C	2.4945	-2.8002	-2.4945
H	4.1546	-1.6313	-1.7628

H	0.6406	-3.7626	-3.0170
H	3.1119	-3.4678	-3.0896
C	-1.5699	-0.4891	0.1229
C	-2.4179	-0.3911	-1.0006
C	-2.1638	-1.0062	1.2856
C	-3.7522	-0.7935	-0.9775
H	-2.0139	0.0202	-1.9258
C	-3.5038	-1.4109	1.3307
H	-1.5713	-1.0920	2.1938
C	-4.3066	-1.3107	0.1970
H	-4.3634	-0.6999	-1.8722
H	-3.9186	-1.8009	2.2575
H	-5.3472	-1.6225	0.2261
C	0.7196	0.0369	1.4866
C	1.0811	1.2042	2.1787
C	1.0248	-1.1760	2.1395
C	1.6950	1.1736	3.4371
H	0.8896	2.1740	1.7248
C	1.6298	-1.2275	3.3941

H	0.7826	-2.1139	1.6394
C	1.9703	-0.0437	4.0552
H	1.9612	2.1059	3.9302
H	1.8424	-2.1890	3.8559
H	2.4473	-0.0735	5.0312

BP-DMPT Singlet Excited State

ZPE = -1019.81

N	4.3428	-0.3260	0.2180
C	3.8642	-1.0276	1.4590
H	2.8923	-0.6174	1.7311
H	3.7852	-2.0963	1.2670
H	4.5920	-0.8380	2.2481
C	4.3123	1.1431	0.5008
H	4.5949	1.6918	-0.3970
H	3.2969	1.4059	0.7918
H	4.9989	1.3562	1.3197
C	3.4242	-0.6334	-0.9829

H	3.9030	-0.1351	-1.8290
H	3.4827	-1.7129	-1.1242
C	2.0015	-0.1912	-0.8169
C	1.5813	1.0555	-1.2957
C	1.0504	-1.0354	-0.2235
C	0.2606	1.4612	-1.1752
H	2.2979	1.7157	-1.7788
C	-0.2721	-0.6456	-0.0849
H	1.3537	-2.0144	0.1407
C	-0.6927	0.6147	-0.5646
H	-0.0441	2.4260	-1.5680
H	-0.9773	-1.3094	0.4035
C	-2.0605	1.0616	-0.4216
C	-3.2371	0.2423	-0.0367
C	-3.4200	-1.0435	-0.5729
C	-4.2039	0.7850	0.8269
C	-4.5254	-1.7959	-0.1916
H	-2.7027	-1.4437	-1.2826
C	-5.3154	0.0271	1.1859

H	-4.0677	1.7832	1.2308
C	-5.4759	-1.2641	0.6849
H	-4.6544	-2.7964	-0.5930
H	-6.0542	0.4464	1.8618
H	-6.3423	-1.8539	0.9676
O	-2.3729	2.2897	-0.6758
C	5.7148	-0.8088	-0.1302
C	6.7809	0.0701	-0.2739
C	5.9017	-2.1786	-0.3299
C	8.0401	-0.4319	-0.6118
H	6.6723	1.1370	-0.1284
C	7.1608	-2.6579	-0.6648
H	5.0811	-2.8815	-0.2303
C	8.2547	-1.7944	-0.8109
H	8.8670	0.2645	-0.7184
H	7.2958	-3.7256	-0.8159
C	9.6118	-2.3357	-1.1693
H	9.5722	-2.8872	-2.1137
H	10.3440	-1.5316	-1.2709

H	9.9673	-3.0286	-0.4002

BP-DMPT Triplet Excited State

ZPE = -1019.82

N	4.3604	-0.3238	0.2227
C	3.8928	-1.0231	1.4691
H	2.9239	-0.6115	1.7496
H	3.8104	-2.0918	1.2791
H	4.6281	-0.8335	2.2512
C	4.3309	1.1456	0.5024
H	4.6055	1.6924	-0.3991
H	3.3179	1.4083	0.8020
H	5.0249	1.3614	1.3142
C	3.4304	-0.6351	-0.9699
H	3.8987	-0.1336	-1.8201
H	3.4943	-1.7143	-1.1120
C	2.0076	-0.2027	-0.7883
C	1.5732	1.0473	-1.2539

C	1.0670	-1.0591	-0.1915
C	0.2530	1.4412	-1.1196
H	2.2806	1.7148	-1.7403
C	-0.2549	-0.6815	-0.0376
H	1.3830	-2.0367	0.1653
C	-0.6974	0.5797	-0.5113
H	-0.0628	2.4043	-1.5091
H	-0.9485	-1.3496	0.4611
C	-2.0497	1.0117	-0.3500
C	-3.2374	0.2282	-0.0122
C	-3.4008	-1.0845	-0.4949
C	-4.2636	0.8137	0.7556
C	-4.5431	-1.8056	-0.1711
H	-2.6432	-1.5240	-1.1362
C	-5.4085	0.0850	1.0606
H	-4.1466	1.8259	1.1303
C	-5.5501	-1.2267	0.6070
H	-4.6576	-2.8197	-0.5416
H	-6.1894	0.5415	1.6608

H	-6.4428	-1.7941	0.8505
O	-2.3158	2.2974	-0.5374
C	5.7295	-0.8056	-0.1370
C	6.7920	0.0750	-0.2959
C	5.9175	-2.1760	-0.3326
C	8.0487	-0.4254	-0.6452
H	6.6823	1.1423	-0.1542
C	7.1741	-2.6537	-0.6787
H	5.0996	-2.8804	-0.2213
C	8.2643	-1.7883	-0.8406
H	8.8726	0.2724	-0.7640
H	7.3102	-3.7218	-0.8266
C	9.6186	-2.3280	-1.2121
H	9.5699	-2.8815	-2.1550
H	10.3483	-1.5230	-1.3229
H	9.9830	-3.0190	-0.4454

Reduced BP-DMPT

ZPE = -1020.03

N	4.3343	-0.3546	0.2064
C	3.8171	-1.0851	1.4099
H	2.8350	-0.6820	1.6544
H	3.7371	-2.1483	1.1892
H	4.5154	-0.9192	2.2312
C	4.2826	1.1049	0.5152
H	4.5777	1.6731	-0.3666
H	3.2562	1.3499	0.7818
H	4.9472	1.3132	1.3540
C	3.4121	-0.6402	-1.0441
H	3.9273	-0.1153	-1.8530
H	3.5048	-1.7173	-1.1917
C	2.0040	-0.2126	-0.8919
C	1.5764	1.0715	-1.3054
C	1.0277	-1.0685	-0.3264
C	0.2702	1.4813	-1.1532
H	2.2988	1.7489	-1.7598
C	-0.2854	-0.6732	-0.1733

H	1.3217	-2.0637	0.0047
C	-0.7285	0.6231	-0.5874
H	-0.0386	2.4702	-1.4757
H	-0.9811	-1.3593	0.2981
C	-2.0611	1.1474	-0.4179
C	-3.1984	0.2636	-0.0127
C	-3.3782	-1.0458	-0.4894
C	-4.1931	0.8032	0.8205
C	-4.4945	-1.7957	-0.1213
H	-2.6560	-1.4712	-1.1804
C	-5.3023	0.0519	1.1980
H	-4.0764	1.8272	1.1627
C	-5.4581	-1.2561	0.7322
H	-4.6181	-2.8018	-0.5131
H	-6.0513	0.4876	1.8539
H	-6.3260	-1.8421	1.0202
O	-2.3068	2.3799	-0.5848
C	5.7081	-0.8199	-0.1211
C	6.7687	0.0688	-0.2558

C	5.9142	-2.1866	-0.3292
C	8.0355	-0.4174	-0.5879
H	6.6466	1.1338	-0.1059
C	7.1802	-2.6515	-0.6587
H	5.0991	-2.8969	-0.2420
C	8.2664	-1.7767	-0.7923
H	8.8558	0.2880	-0.6863
H	7.3266	-3.7169	-0.8164
C	9.6327	-2.3019	-1.1416
H	9.6030	-2.8737	-2.0743
H	10.3508	-1.4874	-1.2602
H	10.0015	-2.9721	-0.3583

Oxidized Tetraphenyl Borate

ZPE = -950.66

B	0.0000	0.0026	0.0020
C	-0.0172	1.5080	-0.6721
C	-0.8754	2.4955	-0.1441

C	0.7659	1.9094	-1.7665
C	-0.9394	3.7915	-0.6530
H	-1.5206	2.2332	0.6946
C	0.7119	3.2047	-2.2961
H	1.4369	1.1917	-2.2336
C	-0.1392	4.1564	-1.7397
H	-1.6162	4.5172	-0.2077
H	1.3349	3.4652	-3.1488
H	-0.1856	5.1630	-2.1466
C	0.8700	-1.0468	-0.9276
C	2.2741	-0.9237	-0.9856
C	0.3231	-2.0970	-1.6827
C	3.0759	-1.7696	-1.7502
H	2.7548	-0.1374	-0.4033
C	1.1117	-2.9605	-2.4533
H	-0.7524	-2.2598	-1.6683
C	2.4945	-2.8002	-2.4945
H	4.1546	-1.6313	-1.7628
H	0.6406	-3.7626	-3.0170

H	3.1119	-3.4678	-3.0896
C	-1.5699	-0.4891	0.1229
C	-2.4179	-0.3911	-1.0006
C	-2.1638	-1.0062	1.2856
C	-3.7522	-0.7935	-0.9775
H	-2.0139	0.0202	-1.9258
C	-3.5038	-1.4109	1.3307
H	-1.5713	-1.0920	2.1938
C	-4.3066	-1.3107	0.1970
H	-4.3634	-0.6999	-1.8722
H	-3.9186	-1.8009	2.2575
H	-5.3472	-1.6225	0.2261
C	0.7196	0.0369	1.4866
C	1.0811	1.2042	2.1787
C	1.0248	-1.1760	2.1395
C	1.6950	1.1736	3.4371
H	0.8896	2.1740	1.7248
C	1.6298	-1.2275	3.3941
H	0.7826	-2.1139	1.6394

C	1.9703	-0.0437	4.0552
H	1.9612	2.1059	3.9302
H	1.8424	-2.1890	3.8559
H	2.4473	-0.0735	5.0312

Phenyl Radical

ZPE = -231.39

C	-1.2132	0.6264	0.0000
C	-1.2256	-0.7754	0.0000
C	-0.0000	-1.4039	0.0000
C	1.2255	-0.7754	0.0000
C	1.2132	0.6264	0.0000
C	0.0000	1.3179	0.0000
H	-2.1524	1.1725	0.0000
H	-2.1606	-1.3276	0.0000
H	2.1606	-1.3277	0.0000
H	2.1524	1.1725	0.0000
H	0.0000	2.4036	0.0000

Triphenyl Borane

ZPE = -719.29

B	0.0011	0.0003	-0.0012
C	0.2049	1.5560	-0.0012
C	1.3001	2.1499	0.6545
C	-0.7012	2.4119	-0.6560
C	1.4751	3.5326	0.6716
H	2.0188	1.5183	1.1714
C	-0.5165	3.7934	-0.6701
H	-1.5575	1.9865	-1.1740
C	0.5695	4.3564	0.0016
H	2.3191	3.9677	1.1989
H	-1.2209	4.4310	-1.1964
H	0.7099	5.4336	0.0029
C	-1.4483	-0.6008	-0.0005
C	-2.5089	0.0483	0.6598
C	-1.7384	-1.8097	-0.6614
C	-3.7946	-0.4897	0.6746
H	-2.3196	0.9834	1.1818

C	-3.0280	-2.3383	-0.6781
H	-0.9427	-2.3369	-1.1826
C	-4.0575	-1.6814	-0.0024
H	-4.5923	0.0220	1.2053
H	-3.2298	-3.2638	-1.2097
H	-5.0613	-2.0967	-0.0035
C	1.2459	-0.9550	-0.0010
C	1.2126	-2.1971	0.6609
C	2.4387	-0.6035	-0.6612
C	2.3211	-3.0419	0.6789
H	0.3074	-2.4996	1.1823
C	3.5412	-1.4564	-0.6746
H	2.4986	0.3481	-1.1841
C	3.4858	-2.6751	0.0031
H	2.2757	-3.9875	1.2114
H	4.4442	-1.1695	-1.2057
H	4.3475	-3.3367	0.0047

Phenyl Radical added to Methacrylate

ZPE = -616.26

C	-1.3329	0.5168	-0.6571
H	-0.7206	-0.3484	-0.3953
C	-0.5191	1.7738	-0.5967
C	0.7838	1.8273	0.0481
O	1.4421	2.8520	0.1759
O	1.2135	0.6246	0.4919
C	2.4725	0.6069	1.1867
H	2.8126	-0.4274	1.1087
H	3.1779	1.2576	0.6645
C	2.3026	1.0218	2.6351
H	3.2655	0.9569	3.1507
H	1.9427	2.0514	2.7061
H	1.5953	0.3604	3.1439
C	-1.1135	3.0438	-1.0946
H	-1.8040	3.4643	-0.3487
H	-0.3449	3.7929	-1.2917
H	-1.6977	2.8656	-2.0037
H	-1.6976	0.3802	-1.6828

C	-2.5279	0.6082	0.2790
C	-3.8240	0.7724	-0.2148
C	-2.3313	0.5691	1.6647
C	-4.9079	0.8875	0.6580
H	-3.9863	0.8072	-1.2895
C	-3.4108	0.6823	2.5380
H	-1.3239	0.4465	2.0577
C	-4.7041	0.8424	2.0360
H	-5.9106	1.0116	0.2592
H	-3.2438	0.6455	3.6106
H	-5.5461	0.9305	2.7160

Benzophenone anion after HM2

ZPE = -615.00

C	3.3192	-0.6700	-0.6819
H	4.1030	-0.0207	-1.0614
H	3.6030	-1.6683	-0.3607
C	2.0197	-0.2445	-0.6087
C	1.6025	1.0878	-1.0278

C	0.9404	-1.0798	-0.1016
C	0.3030	1.4974	-0.9630
H	2.3666	1.7656	-1.4044
C	-0.3577	-0.6533	-0.0559
H	1.1918	-2.0753	0.2591
C	-0.7517	0.6497	-0.4956
H	0.0342	2.5009	-1.2847
H	-1.1068	-1.3254	0.3559
C	-2.0910	1.1606	-0.4360
C	-3.2344	0.2244	-0.1157
C	-3.4123	-0.9945	-0.7800
C	-4.1949	0.6334	0.8168
C	-4.5235	-1.7936	-0.5081
H	-2.6868	-1.3106	-1.5247
C	-5.2941	-0.1725	1.1053
H	-4.0675	1.5913	1.3133
C	-5.4621	-1.3895	0.4413
H	-4.6562	-2.7315	-1.0399
H	-6.0234	0.1498	1.8432

H	-6.3230	-2.0153	0.6583
O	-2.3877	2.3567	-0.6364

Oxidized DMPT Amine

ZPE = -404.98

C	0.5502	-1.2313	-0.0278
C	1.9241	-1.2153	-0.0312
C	2.6462	-0.0038	0.0341
C	1.9227	1.2100	0.0929
C	0.5507	1.2269	0.0880
C	-0.1803	-0.0027	0.0310
H	0.0252	-2.1761	-0.0943
H	2.4688	-2.1526	-0.0890
H	2.4683	2.1475	0.1465
H	0.0252	2.1718	0.1492
N	-1.5262	-0.0026	0.0314
C	-2.2824	-1.2525	0.1189
H	-1.8832	-1.8766	0.9199

H	-3.3215	-1.0150	0.3345
H	-2.2251	-1.7902	-0.8330
C	-2.2820	1.2476	-0.0543
H	-1.8861	1.8705	-0.8578
H	-3.3223	1.0106	-0.2645
H	-2.2197	1.7864	0.8967
C	4.1391	0.0039	0.0694
H	4.4811	0.1705	1.0988
H	4.5524	-0.9459	-0.2749
H	4.5412	0.8182	-0.5397

Ionic Complex between Benzophenone Anion and Oxidized DMPT

ZPE = -1020.06

C	3.0859	-0.1839	-1.3148
H	3.7597	0.5639	-1.7182
H	3.4698	-1.1834	-1.1422
C	1.7512	0.1398	-1.0125
C	1.2398	1.4461	-1.2577

C	0.8569	-0.8283	-0.4776
C	-0.0851	1.7438	-1.0197
H	1.9072	2.2035	-1.6606
C	-0.4724	-0.5225	-0.2500
H	1.2315	-1.8238	-0.2546
C	-0.9715	0.7621	-0.5365
H	-0.4712	2.7382	-1.2237
H	-1.1274	-1.2806	0.1678
C	-2.3915	1.1516	-0.3216
C	-3.4637	0.1031	-0.2601
C	-3.4305	-1.0493	-1.0530
C	-4.5604	0.3300	0.5801
C	-4.4801	-1.9649	-1.0021
H	-2.5999	-1.2106	-1.7341
C	-5.5996	-0.5941	0.6441
H	-4.5849	1.2337	1.1815
C	-5.5612	-1.7426	-0.1489
H	-4.4561	-2.8489	-1.6325
H	-6.4407	-0.4180	1.3077

H	-6.3751	-2.4604	-0.1051
O	-2.6950	2.3296	-0.1747
C	-0.5113	-0.4324	-3.9195
C	0.8243	-0.5845	-4.2669
C	1.5918	0.4937	-4.7279
C	0.9557	1.7304	-4.8347
C	-0.3883	1.8988	-4.4928
C	-1.1477	0.8192	-4.0170
H	-1.0580	-1.2847	-3.5258
H	1.2930	-1.5596	-4.1481
H	1.5189	2.5924	-5.1867
H	-0.8326	2.8835	-4.5876
N	-2.4788	0.9596	-3.5753
C	-3.4445	0.0360	-4.1617
H	-3.0764	-0.9904	-4.1322
H	-4.3745	0.0786	-3.5877
H	-3.6655	0.2961	-5.2105
C	-3.0053	2.3100	-3.5055
H	-3.1473	2.7669	-4.5000

H	-3.9746	2.2772	-3.0010
H	-2.3408	2.9457	-2.9146
C	3.0439	0.3173	-5.0934
H	3.6258	1.2105	-4.8465
H	3.4814	-0.5329	-4.5609
H	3.1650	0.1322	-6.1671

Benzophenone Radical

ZPE = -614.87

C	3.2958	-0.7006	-0.8231
H	4.0324	-0.0866	-1.3290
H	3.6065	-1.6659	-0.4398
C	1.9725	-0.2551	-0.6671
C	1.5587	1.0150	-1.1651
C	0.9985	-1.0531	-0.0030
C	0.2603	1.4495	-1.0050
H	2.2867	1.6416	-1.6732

C	-0.3060	-0.6177	0.1354
H	1.2960	-2.0170	0.4006
C	-0.6978	0.6379	-0.3661
H	-0.0455	2.4230	-1.3760
H	-1.0238	-1.2417	0.6589
C	-2.0714	1.1807	-0.1840
C	-3.2309	0.2466	-0.0088
C	-3.3136	-0.9721	-0.6921
C	-4.2887	0.6529	0.8129
C	-4.4443	-1.7753	-0.5511
H	-2.5091	-1.2830	-1.3523
C	-5.4064	-0.1609	0.9700
H	-4.2209	1.6072	1.3266
C	-5.4859	-1.3757	0.2859
H	-4.5115	-2.7121	-1.0956
H	-6.2175	0.1522	1.6202
H	-6.3614	-2.0076	0.4017
O	-2.2621	2.3902	-0.1739

DMPT Amine

ZPE = -405.17

C	0.5423	-1.2036	-0.0677
C	1.9314	-1.1887	-0.0021
C	2.6617	0.0045	0.0223
C	1.9298	1.1924	-0.0209
C	0.5373	1.2026	-0.0873
C	-0.1950	-0.0007	-0.1262
H	0.0340	-2.1603	-0.0811
H	2.4615	-2.1386	0.0347
H	2.4562	2.1442	0.0023
H	0.0279	2.1584	-0.1128
N	-1.5826	-0.0075	-0.2364
C	-2.2841	-1.2307	0.1151
H	-2.0744	-1.5540	1.1470
H	-3.3568	-1.0603	0.0163
H	-2.0150	-2.0449	-0.5634

C	-2.2899	1.2328	0.0297
H	-1.9919	2.0096	-0.6798
H	-3.3589	1.0614	-0.1019
H	-2.1152	1.6085	1.0506
C	4.1658	-0.0037	0.1287
H	4.4922	-0.3165	1.1274
H	4.6112	-0.6972	-0.5915
H	4.5788	0.9914	-0.0583

Benzophenone Radical added to Methacrylate

ZPE = -999.71

C	-0.8398	-0.0484	-0.5528
H	-0.4890	-0.9101	0.0244
C	0.2407	0.9737	-0.6876
C	1.1167	1.2859	0.4295
O	1.9870	2.1476	0.4124
O	0.8768	0.5106	1.5120
C	1.6483	0.7911	2.6923

H	1.6024	-0.1314	3.2743
H	2.6849	0.9831	2.4056
C	1.0601	1.9569	3.4629
H	1.6290	2.1136	4.3843
H	1.1017	2.8755	2.8722
H	0.0192	1.7531	3.7313
C	0.3734	1.7446	-1.9518
H	1.0969	2.5552	-1.8573
H	0.6908	1.0829	-2.7695
H	-0.5981	2.1606	-2.2497
H	-1.1333	-0.4020	-1.5478
C	-2.0864	0.5414	0.1546
H	-2.4536	1.3977	-0.4213
H	-1.7889	0.9042	1.1440
C	-3.1754	-0.4907	0.2918
C	-4.1585	-0.6336	-0.6956
C	-3.1924	-1.3616	1.3868
C	-5.1328	-1.6196	-0.5910
H	-4.1572	0.0368	-1.5518

C	-4.1788	-2.3365	1.5096
H	-2.4262	-1.2701	2.1533
C	-5.1591	-2.4720	0.5192
H	-5.8888	-1.7336	-1.3622
H	-4.1710	-3.0040	2.3663
C	-6.2039	-3.5409	0.5707
C	-6.7067	-4.0280	1.8954
C	-6.8070	-3.1826	3.0065
C	-7.1465	-5.3538	1.9913
C	-7.3420	-3.6619	4.2012
H	-6.4904	-2.1464	2.9338
C	-7.6595	-5.8360	3.1913
H	-7.0762	-5.9971	1.1193
C	-7.7595	-4.9890	4.2972
H	-7.4320	-2.9987	5.0560
H	-7.9857	-6.8689	3.2651
H	-8.1664	-5.3631	5.2319
O	-6.6490	-4.0158	-0.4634

Benzoyl Peroxide

ZPE = -839.85

C	5.5278	-0.3208	-0.0440
C	4.9773	0.5965	-0.9406
C	3.6125	0.8622	-0.9114
C	2.7984	0.2075	0.0185
C	3.3469	-0.7136	0.9181
C	4.7141	-0.9736	0.8824
H	6.5934	-0.5281	-0.0681
H	5.6109	1.1028	-1.6617
H	3.1677	1.5716	-1.6018
H	2.7171	-1.2249	1.6378
H	5.1436	-1.6876	1.5777
C	1.3501	0.5364	-0.0055
C	-1.3501	-0.5367	-0.0053
C	-2.7984	-0.2077	0.0184
C	-3.3469	0.7139	0.9176

C	-3.6125	-0.8628	-0.9112
C	-4.7141	0.9739	0.8817
H	-2.7171	1.2255	1.6370
C	-4.9773	-0.5970	-0.9406
H	-3.1678	-1.5725	-1.6013
C	-5.5278	0.3208	-0.0444
H	-5.1435	1.6883	1.5767
H	-5.6110	-1.1036	-1.6614
H	-6.5934	0.5282	-0.0686
O	0.7984	1.2962	-0.7524
O	-0.7985	-1.2968	-0.7520
O	0.6829	-0.1582	0.9807
O	-0.6830	0.1582	0.9807

Benzoic Acid

ZPE = -420.57

C	-1.3954	-0.5241	-0.0576
C	-2.8494	-0.2122	-0.0097

C	-3.3625	0.7594	0.8555
C	-3.7027	-0.9221	-0.8597
C	-4.7311	1.0173	0.8669
H	-2.6960	1.3071	1.5129
C	-5.0691	-0.6602	-0.8445
H	-3.2852	-1.6720	-1.5240
C	-5.5832	0.3092	0.0187
H	-5.1325	1.7705	1.5376
H	-5.7331	-1.2103	-1.5038
H	-6.6497	0.5129	0.0301
O	-0.8930	-1.3561	-0.7819
O	-0.6658	0.2154	0.7941
H	0.2640	-0.0518	0.6983

Benzoloxy Radical

ZPE = -419.90

C	-1.4226	-0.5318	-0.0433
C	-2.8650	-0.2257	-0.0108

C	-3.3630	0.7501	0.8576
C	-3.7146	-0.9326	-0.8656
C	-4.7282	1.0190	0.8680
H	-2.6935	1.2935	1.5194
C	-5.0780	-0.6576	-0.8490
H	-3.3024	-1.6851	-1.5311
C	-5.5820	0.3159	0.0162
H	-5.1261	1.7738	1.5383
H	-5.7477	-1.1998	-1.5084
H	-6.6468	0.5279	0.0266
O	-0.8531	-1.3647	-0.7336
O	-0.6113	0.1420	0.7432

DMPT Aminoalkyl Radical

ZPE = -404.53

C	0.5385	-1.1869	-0.1465
C	1.9286	-1.1761	-0.1113

C	2.6555	0.0075	0.0616
C	1.9245	1.1896	0.2106
C	0.5328	1.2045	0.1832
C	-0.1891	0.0109	-0.0042
H	0.0244	-2.1296	-0.2958
H	2.4615	-2.1176	-0.2268
H	2.4536	2.1273	0.3655
H	0.0105	2.1411	0.3412
N	-1.5837	0.0102	-0.0410
C	-2.2932	-1.2565	0.0628
H	-1.8962	-1.8517	0.8896
H	-3.3461	-1.0502	0.2544
H	-2.2112	-1.8344	-0.8654
C	-2.3142	1.1636	-0.1957
H	-1.8326	2.0313	-0.6254
H	-3.3879	1.0540	-0.2515
C	4.1626	0.0018	0.0697
H	4.5572	0.9411	0.4664
H	4.5535	-0.8170	0.6817

H	4.5632	-0.1264	-0.9424

Benzoloxy Radical added to Methacrylate

ZPE = -804.74

C	-0.7264	0.0567	0.4793
H	-0.1568	-0.3774	1.3036
C	-0.2962	1.4587	0.1872
C	1.0898	1.8511	0.3830
O	1.5315	2.9657	0.1440
O	1.8535	0.8392	0.8495
C	3.2351	1.1429	1.1205
H	3.7327	0.1715	1.1098
H	3.6290	1.7575	0.3076
C	3.3922	1.8280	2.4633
H	4.4543	1.9969	2.6646
H	2.8826	2.7947	2.4710
H	2.9849	1.2036	3.2636

C	-1.2636	2.4139	-0.4084
H	-2.0597	2.6586	0.3051
H	-0.7631	3.3333	-0.7133
H	-1.7583	1.9639	-1.2797
H	-0.5707	-0.5674	-0.4110
O	-2.1141	0.0708	0.8492
C	-3.0573	-0.5904	0.1448
C	-2.6910	-1.8893	-0.4997
C	-3.3182	-2.2327	-1.7002
C	-1.8130	-2.7860	0.1178
C	-3.0476	-3.4617	-2.2960
H	-4.0116	-1.5338	-2.1580
C	-1.5623	-4.0231	-0.4704
H	-1.3418	-2.5284	1.0625
C	-2.1720	-4.3573	-1.6804
H	-3.5245	-3.7237	-3.2352
H	-0.8923	-4.7256	0.0151
H	-1.9681	-5.3189	-2.1417
O	-4.1804	-0.1453	0.1143

DMPT Aminoaklyl Radical added to Methacrylate

ZPE = -789.37

C	-1.2511	0.1113	-0.3323
H	-0.4462	-0.6120	-0.1902
C	-0.6957	1.4971	-0.3662
C	0.5501	1.8428	0.2990
O	1.0106	2.9771	0.3349
O	1.1629	0.7850	0.8758
C	2.3769	1.0574	1.5965
H	2.8905	0.0950	1.6393
H	2.9827	1.7625	1.0223
C	2.0816	1.5841	2.9872
H	3.0198	1.7280	3.5317
H	1.5614	2.5439	2.9381
H	1.4654	0.8725	3.5445
C	-1.4674	2.6107	-0.9862
H	-1.8349	3.3097	-0.2227

H	-0.8357	3.1998	-1.6603
H	-2.3254	2.2284	-1.5437
H	-1.7529	-0.1036	-1.2841
C	-2.2919	-0.0162	0.7962
H	-3.0071	0.8068	0.7005
H	-1.7768	0.0960	1.7682
C	-2.1636	-2.4423	0.7862
H	-2.7588	-3.3511	0.8603
H	-1.5550	-2.5162	-0.1174
H	-1.4932	-2.3949	1.6608
N	-3.0332	-1.2673	0.7228
C	-4.2031	-1.3412	1.5165
C	-5.0902	-2.4204	1.3341
C	-4.5535	-0.3658	2.4589
C	-6.2621	-2.5157	2.0699
H	-4.8656	-3.1770	0.5881
C	-5.7456	-0.4691	3.1842
H	-3.9032	0.4806	2.6485
C	-6.6192	-1.5398	3.0131

H	-6.9270	-3.3597	1.8981
H	-5.9866	0.3073	3.9068
C	-7.9029	-1.6547	3.7946
H	-8.7720	-1.6634	3.1280
H	-7.9300	-2.5819	4.3769
H	-8.0181	-0.8173	4.4877

Ethyl Methacrylate

ZPE = -384.81

C	-1.2326	0.4394	0.0538
H	-0.6860	-0.4692	0.2821
H	-2.3032	0.3583	-0.1140
C	-0.6224	1.6258	-0.0212
C	0.8513	1.7474	0.2110
O	1.4388	2.8099	0.1713
O	1.4568	0.5793	0.4577

C	2.8729	0.6232	0.7245
H	3.2197	-0.3884	0.5076
H	3.3426	1.3221	0.0287
C	3.1450	1.0023	2.1662
H	4.2224	0.9701	2.3538
H	2.7888	2.0130	2.3799
H	2.6558	0.3002	2.8472
C	-1.3241	2.9163	-0.3310
H	-1.1965	3.6343	0.4850
H	-0.9074	3.3793	-1.2309
H	-2.3910	2.7420	-0.4851