

Supporting Information

Toward Rational Design of Organic Catalysts for Organocatalysed Atom Transfer Polymerisation

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S1. Excited-State Redox Potentials

The oxidation potentials $E^0(\text{PC}^{\bullet+}/{}^1,{}^3\text{PC}^*)$ of the lowest singlet/triplet excited state ${}^1,{}^3\text{PC}^*$ of a photocatalyst (PC) can be calculated as

$$E^0(\text{PC}^{\bullet+}/{}^1,{}^3\text{PC}^*) = G_{\text{SCE}} - \Delta G(\text{PC}^{\bullet+}/{}^1,{}^3\text{PC}^*) \approx G_{\text{SCE}} - \Delta E(\text{PC}^{\bullet+}/{}^1,{}^3\text{PC}^*), \quad (\text{S1})$$

$$\Delta E(\text{PC}^{\bullet+}/{}^1,{}^3\text{PC}^*) = E({}^1,{}^3\text{PC}^*) - E(\text{PC}^{\bullet+}), \quad (\text{S2})$$

where $G_{\text{SCE}} = -4.60 \text{ eV}^{1,2}$ is the reduction Gibbs free energy of the saturated calomel electrode, whereas $E({}^1,{}^3\text{PC}^*)$ and $E(\text{PC}^{\bullet+})$ are the electronic energies of ${}^1,{}^3\text{PC}^*$ and $\text{PC}^{\bullet+}$ at their equilibrium geometries, respectively. Time-dependent density functional theory (TD-DFT) is used herein in conjunction with the def2-SVP basis set³ and the density-based implicit solvation model (SMD).⁴ To check the accuracy of density functionals, B3LYP^{5,6} with the D3BJ⁷ dispersion correction (B3LYP-D3BJ), PBE0⁸-D3BJ, M06-2X⁹ with the D3¹⁰

dispersion correction (M06-2X-D3), CAM-B3LYP¹¹-D3BJ, and ω B97X-D3¹² are compared. The results, calculated with the same solvents as used in the experimental measurements, are shown in Table S1. As compared to the experimental $E^0(\text{PC}^+/\text{}^1\text{PC}^*)$ [$E^0(\text{PC}^+/\text{}^3\text{PC}^*)$], B3LYP-D3BJ and PBE0-D3BJ result in the smallest errors on average, being 0.18 (0.15) and 0.19 (0.19) eV, respectively. PBE0-D3BJ/def2-SVP/SMD is then used throughout. For a direct comparison of PCs, it is more meaningful to calculate $E^0(\text{PC}^+/\text{}^1,3\text{PC}^*)$ with the solvents commonly used for O-ATRP, i.e., N,N-dimethylformamide (DMF) and N,N-dimethylacetamide (DMAc). As shown in Table S2, the results with DMF are virtually the same as those with DMAc, and thus DMF is used as a representative throughout this work.

Table S1: Experimental and calculated excited-state oxidation potentials (in eV; relative to the saturated calomel electrode) for PC1-5.

catalyst	solvent	$E^0(\text{PC}^+/\text{}^1\text{PC}^*)/E^0(\text{PC}^+/\text{}^3\text{PC}^*)^a$					
		experiment	B3LYP ^b	PBE0 ^b	M06-2X ^c	CAM-B3LYP ^b	ω B97X-D3 ^d
PC1	cyclohexane	-1.92/-1.70 ¹³	-2.19/-1.65	-2.17/-1.57	-2.22/-1.66	-2.44/-1.72	-2.43/-1.70
PC2	toluene	-1.87/-0.70 ¹⁴	-1.75/-0.52	-1.70/-0.41	-1.69/-0.50	-1.89/-0.53	-1.87/-0.51
PC3	acetonitrile	-1.58/-1.41 ¹⁵	-1.78/-1.65	-1.77/-1.58	-2.09/-1.65	-2.30/-1.77	-2.39/-1.73
PC4	chloroform	-1.79/-1.76 ^{e 16}	-1.89/-1.89	-1.94/-1.94	-2.53/-2.23	-2.86/-2.39	-3.11/-2.41
PC5	toluene	-1.84 ¹⁷ / –	-2.04/-1.65	-2.03/-1.60	-2.21/-1.73	-2.51/-1.87	-2.59/-1.91
average error ^f		0.00/0.00	0.18/0.15	0.19/0.19	0.42/0.24	0.60/0.30	0.68/0.29

Note: ^aCalculated with TDDFT/PBE0-D3BJ/def2-SVP and the SMD solvation model.

^bDispersion correction D3BJ⁷ is employed. ^cDispersion correction D3¹⁰ is employed. ^d ω B97X-D3 is reoptimized from ω B97X-D with the D3 dispersion correction.¹² ^eDerived from the ground-state oxidation potentials and photoluminescence data in literature.¹⁶ ^fAbsolute difference between the calculated and experimental $E^0(\text{PC}^+/\text{}^1\text{PC}^*)$ [$E^0(\text{PC}^+/\text{}^3\text{PC}^*)$] being averaged over PC1-5 (PC1-4; N.B.: $E^0(\text{PC}^+/\text{}^3\text{PC}^*)$ for PC5 has not been reported).

Apart from TD-DFT, the oxidation potentials $E^0(\text{PC}^+/\text{}^3\text{PC}^*)$ of $^3\text{PC}^*$ can also be calculated by unrestricted DFT (UDFT). The results are shown in Table S3. Out of the five density functionals, PBE0-D3BJ performs the best on average (0.15 eV in error). In view of this, PBE0-D3BJ is also selected as the density functional for calculating the energy barriers $\Delta E^\ddagger$ for dissociative electron transfer of the triplet exciplex $^3\text{PC}^*/\text{R-X}$.

Table S2: Calculated excited-state oxidation potentials (in eV; relative to the saturated calomel electrode) with DMF and DMAc solvents for PC1-5.

catalyst	$E^0(\text{PC}^{\bullet+}/^1\text{PC}^*)/E^0(\text{PC}^{\bullet+}/^3\text{PC}^*)$	
	DMF ^a	DMAc ^b
PC1	-2.91/-2.31	-2.91/-2.32
PC2	-2.12/-1.05	-2.12/-1.05
PC3	-1.77/-1.59	-1.77/-1.59
PC4	-2.22/-2.21	-2.22/-2.21
PC5	-2.52/-2.10	-2.53/-2.10

Note: ^aCalculated by TDDFT/PBE0-D3BJ/def2-SVP/SMD-DMF. ^bCalculated by TDDFT/PBE0-D3BJ/def2-SVP/SMD-DMAc.

Table S3: Calculated triplet-excited-state oxidation potentials (in eV; relative to the saturated calomel electrode) by UDFT for PC1-5.

catalyst	solvent	$E^0(\text{PC}^{\bullet+}/^3\text{PC}^*)^a$				
		B3LYP ^b	PBE0 ^b	M06-2X ^c	CAM-B3LYP ^b	ω B97X-D3 ^d
PC1	cyclohexane	-1.73	-1.66	-1.81	-1.82	-1.78
PC2	toluene	-0.50	-0.37	-0.43	-0.45	-0.41
PC3	acetonitrile	-1.65	-1.53	-1.60	-1.66	-1.59
PC4	chloroform	-1.98	-1.88	-1.95	-2.05	-2.02
PC5	toluene	-1.68	-1.60	-1.73	-1.84	-1.85
average error ^e		0.17	0.15	0.22	0.25	0.23

Note: ^aCalculated with UPBE0-D3BJ/def2-SVP and the SMD solvation model. ^bDispersion correction D3BJ⁷ is employed. ^cDispersion correction D3¹⁰ is employed. ^d ω B97X-D3 is reoptimized from ω B97X-D with the D3 dispersion correction.¹² ^eAbsolute difference between the calculated and experimental $E^0(\text{PC}^{\bullet+}/^3\text{PC}^*)$ being averaged over PC1-5.

S2. Energy Difference between S₁ and T₁

The adiabatic energy difference $\Delta E_{\text{ST}}^{\text{ad}}$ between S₁ and T₁, which equals to $-[E^0(\text{PC}^{*+}/^1\text{PC}^*) - E^0(\text{PC}^{*+}/^3\text{PC}^*)]$, are listed in Table S4 for PC1-5. It is interesting to notice that the $\Delta E_{\text{ST}}^{\text{ad}}$ for PC2 (1.06 eV) is notably larger than those for other PCs. This trend also holds for the vertical energy difference $\Delta E_{\text{ST}}^{\text{vert}}$ (cf. Table S4) which allows for an analysis solely at the S₀ equilibrium geometry: The transition from the highest occupied (HOMO; ψ_{H}) and lowest unoccupied (LUMO; ψ_{L}) molecular orbitals, $\psi_{\text{H}} \rightarrow \psi_{\text{L}}$, is the dominant configuration (contribution > 70%) for both the S₁ and T₁ states of PC1-5 (cf. Table S4), which means that the repulsive interaction $2(\psi_{\text{L}}\psi_{\text{H}}|\psi_{\text{L}}\psi_{\text{H}})$ in ¹PC* but not present in ³PC* can be a good indicator of $\Delta E_{\text{ST}}^{\text{vert}}$, in view of the response kernel of TD-DFT,¹⁸ i.e.,

$$\begin{aligned}\Delta E_{\text{S/T}}^{\text{vert}} &= E_{\text{S}}^* - E_{\text{T}}^* \\ &= 2 \left(\phi_{\text{L}}\phi_{\text{H}} \left| \frac{1}{r_{12}} \right| \phi_{\text{H}}\phi_{\text{L}} \right) + 2c_{\text{xc}} \left(\phi_{\text{L}}\phi_{\text{H}} \left| (f_{\text{xc}}^{\text{S}} - f_{\text{xc}}^{\text{T}})\delta(\vec{r}_1 - \vec{r}_2) \right| \phi_{\text{H}}\phi_{\text{L}} \right) \quad (\text{S3}) \\ &\approx 2 \left(\phi_{\text{L}}\phi_{\text{H}} \left| \frac{1}{r_{12}} \right| \phi_{\text{H}}\phi_{\text{L}} \right),\end{aligned}$$

where E_{S}^* and E_{T}^* are the vertical excitation energies for S₁ and T₁, respectively, c_{xc} is the scaling coefficient denoting the portion of the static exchange-correlation potential included in the chosen hybrid functional, and $f_{\text{xc}}^{\text{S}} - f_{\text{xc}}^{\text{T}}$ is the difference between the exchange-correlation kernels for S₁ and T₁, being a small term. As such, it is not surprising to see that larger $2(\psi_{\text{L}}\psi_{\text{H}}|\psi_{\text{L}}\psi_{\text{H}})$ corresponds to larger $\Delta E_{\text{ST}}^{\text{vert}}$ and $\Delta E_{\text{ST}}^{\text{ad}}$ (cf. Table S4). That is, PC2's largest $\Delta E_{\text{ST}}^{\text{ad}} = 1.06$ eV is attributed to its most significant $2(\psi_{\text{L}}\psi_{\text{H}}|\psi_{\text{L}}\psi_{\text{H}}) = 5.8 \times 10^{-3}$.

Table S4: Adiabatic and vertical energy differences between S_1 and T_1 , dominant configurations of both excitations, and $2(\psi_L\psi_H|\psi_L\psi_H)$ for PC1-5.

catalyst	$\Delta E_{ST}^{ad}{}^a$	$\Delta E_{ST}^{vert}{}^b$	$\phi_H \rightarrow \phi_L$ in S_1/T_1 ^{bc}	$2(\psi_L\psi_H \psi_L\psi_H)$ ^b
PC1	0.59 eV	0.56 eV	95%/78%	1.9×10^{-3}
PC2	1.06 eV	1.21 eV	97%/95%	5.8×10^{-3}
PC3	0.18 eV	0.27 eV	96%/95%	1.3×10^{-3}
PC4	0.01 eV	0.01 eV	93%/92%	4.2×10^{-5}
PC5	0.42 eV	0.42 eV	95%/81%	1.7×10^{-3}

Note: The results are calculated by TDDFT/PBE0-D3BJ/def2-SVP/SMD-DMF. ^aAdiabatic energy difference between S_1 and T_1 , equaling to $-(E^0(PC^{++}/{}^1PC^*) - E^0(PC^{++}/{}^3PC^*))$.

^bCalculated based on the equilibrium geometry of S_0 . ^cThe contribution of the $\phi_H \rightarrow \phi_L$ configuration of S_1 and T_1 excitations, respectively.

S3. Electronic Structure of Lowest Excited States

Clearly, the binding strength ΔE_b^{ex} of the exciplex $^1,^3\text{PC}^*/\text{R}-\text{X}$ (between $^1,^3\text{PC}^*$ and $\text{R}-\text{X}$) is dependent on the electronic structure of $^1,^3\text{PC}^*$. To see this, the excitation types of $^1,^3\text{PC}^*$ for PC1-5 are documented in Fig. S1. The $^3\text{PC}^*$ of PC1 and $^1\text{PC}^*$ of PC2 are all local excitations, with positively charged regions only exist in the vicinity of peripheral phenyl-H atoms (cf. Fig. S2). By contrast, the $^3\text{PC}^*$ of PC3, PC4, and PC5 are all charge-transfer type of excitations (cf. Fig. S1), which renders notable charge separation with half of the molecule positively charged and the other half negatively charged (cf. Fig. S2). Since the charge-separated $^3\text{PC}^*$ and $\text{R}-\text{X}$ are both polar systems, higher ΔE_b^{ex} of $^3\text{PC}^*/\text{R}-\text{X}$ for PC3-5 can be expected (cf. Table 1 in the main text).

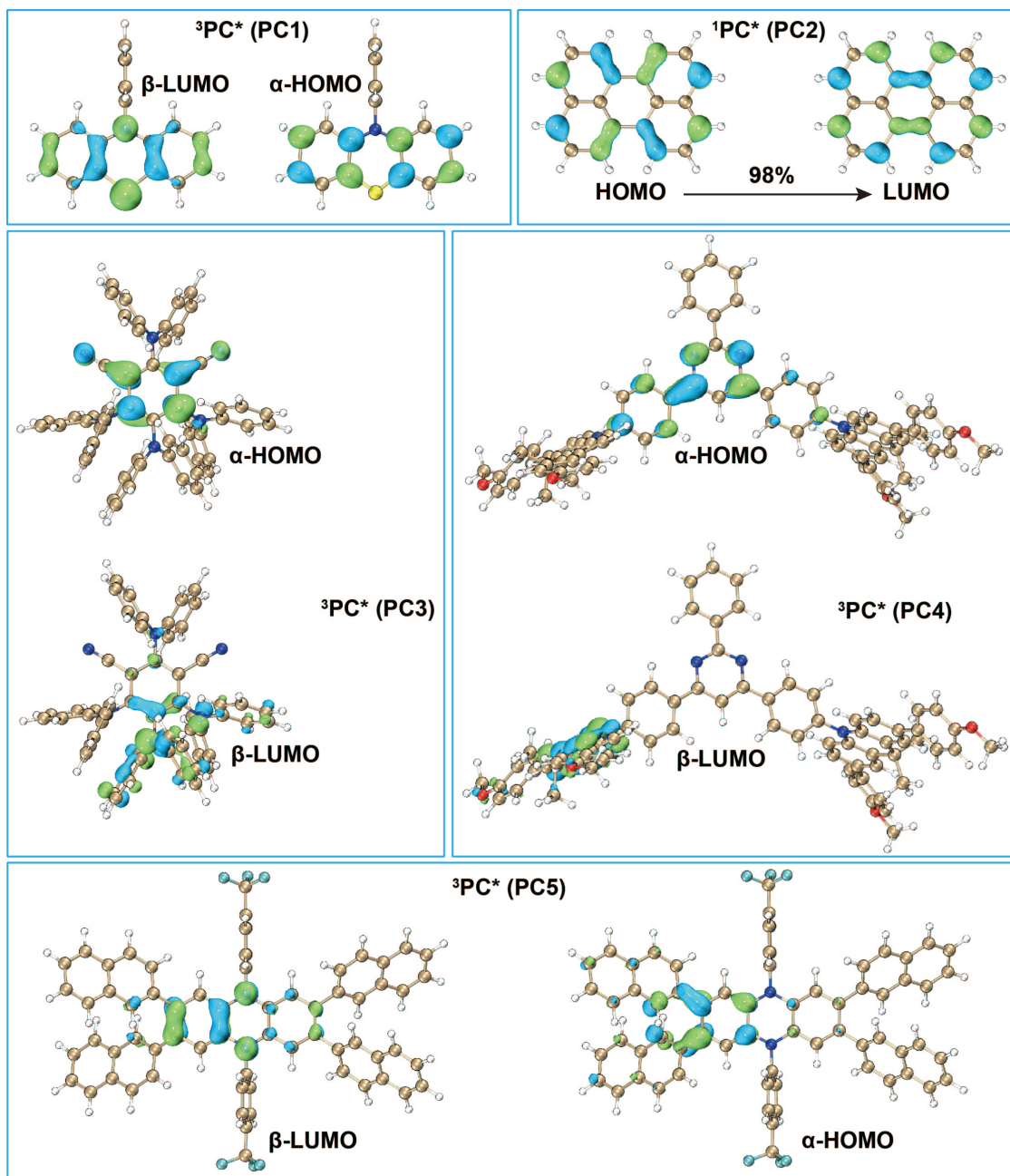


Figure S1: Illustration of the electron and hole of $^3\text{PC}^*$ (represented by the α -HOMO and β -LUMO, respectively) for PC1, PC3, PC4, and PC5, as well as $^1\text{PC}^*$ (represented by the LUMO and HOMO, respectively, in the case of HOMO $\rightarrow$ LUMO-dominated S_1 excitation) for PC2. $^3\text{PC}^*$ and $^1\text{PC}^*$ are calculated by UPBE0/def2-SVP/SMD-DMF and TDDFT/PBE0/def2-SVP/SMD-DMF, respectively.

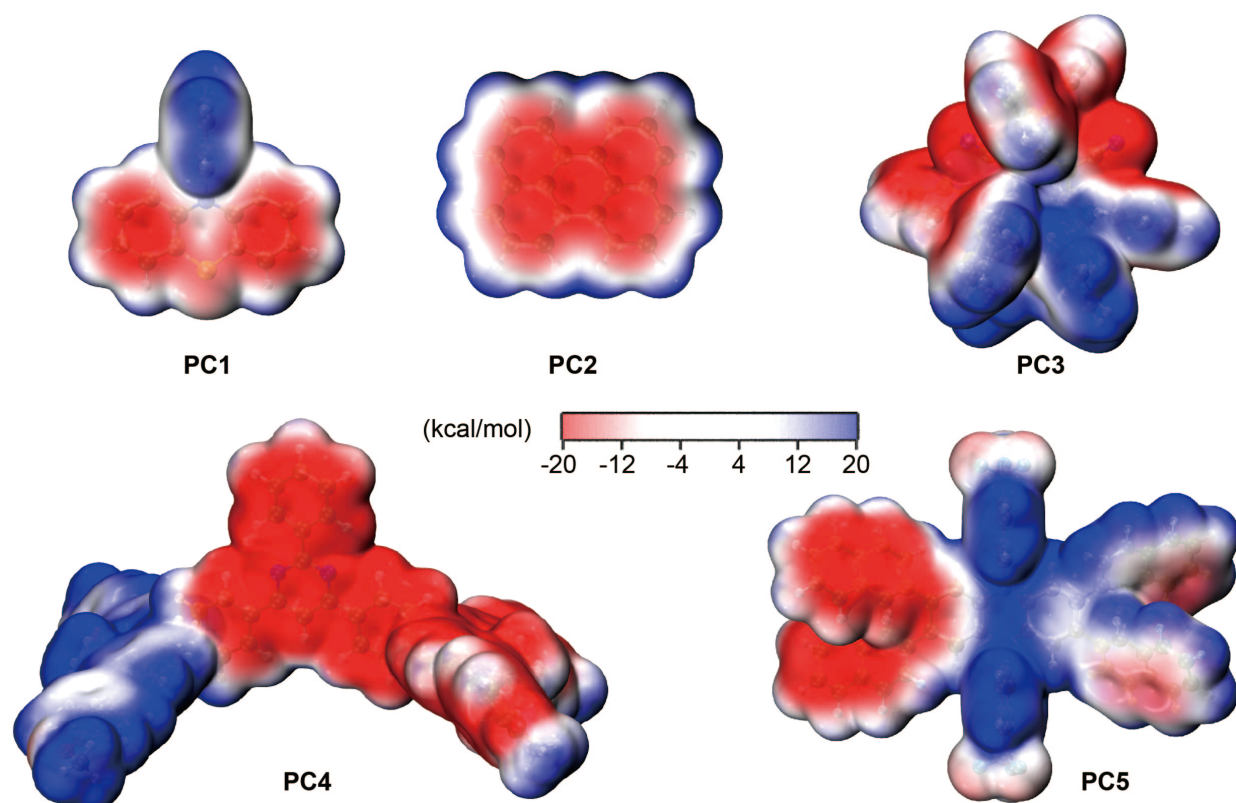


Figure S2: $^3\text{PC}^*$ (PC1, PC3, PC4, and PC5) and $^1\text{PC}^*$ (PC2) electrostatic potential maps^{19,20} on the van Der Waals surfaces at their respective equilibrium geometries, calculated by UPBE0/def2-SVP/SMD-DMF and TDDFT/PBE0/def2-SVP/SMD-DMF, respectively.

S4. Fragment Localized Molecular Orbitals

In the main text, the dissociative electron transfer $^1,^3\text{PC}^*/\text{R}-\text{X} \longrightarrow \text{PC}^{\bullet+}/\text{X}^- + \text{R}^\bullet$ in O-ATRP is studied in detail with PC1 as an example, where fragment localized molecular orbitals (FLMO)²¹ are used to reveal the contributions of individual orbitals to the electron/hole transfer process. The FLMOs are constructed noniteratively in terms of the orthonormal primitive FLMOs from subsystem calculations^{22,23} (phenyl, Br, and acetyl for EBPA; N-phenyl and phenothiazine for PC1) by using the BDF program package.^{24,25} In particular, the localized FLMOs for a conjugated π system can be canonicalized to produce the same number of regional FLMOs (delocalized within the π system). That is, the six phenyl- π/π^* and fourteen phenothiazine- π/π^* localized FLMOs are converted to six (see Fig. S3) and fourteen (see Fig. S4) regional FLMOs, respectively. The so-obtained new FLMOs $\phi_{\text{R},p}^{\text{FLMO}}$, still being orthonormal, can be used to expand the occupied spin orbitals $\{\phi_{\text{R},i\sigma}^{\text{FLMO}}\}$ of $^3\text{PC}^*/\text{R}-\text{X}$ with coefficients $C_{pi}^\sigma(\text{R})$. The coefficients for the six phenyl- π/π^* (and fourteen phenothiazine- π/π^* as well) are summed up for analysis (i.e., π/π^* orbitals of a conjugated system are discussed as a whole), in order to simplify the discussion.

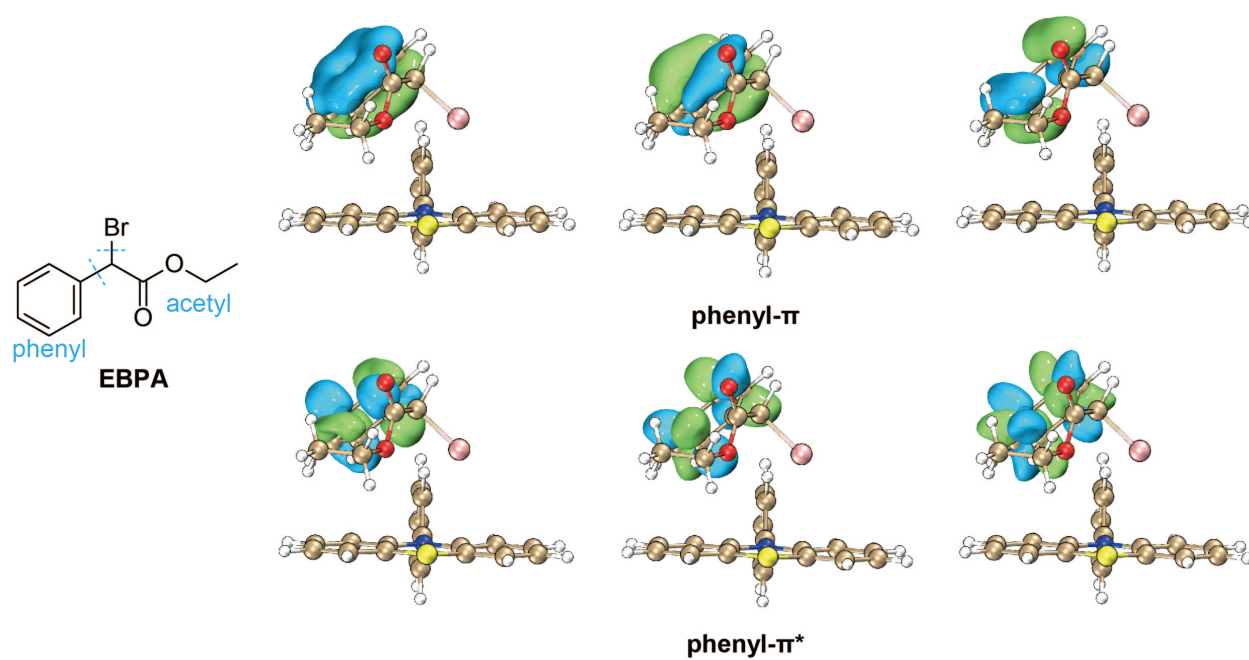


Figure S3: Ground-state (S_0) regional FLMOs corresponding to the six phenyl- π/π^* of PC/R-X but at the equilibrium geometry of $^3\text{PC}^*/\text{R-X}$, calculated by PBE0/def2-SVP.

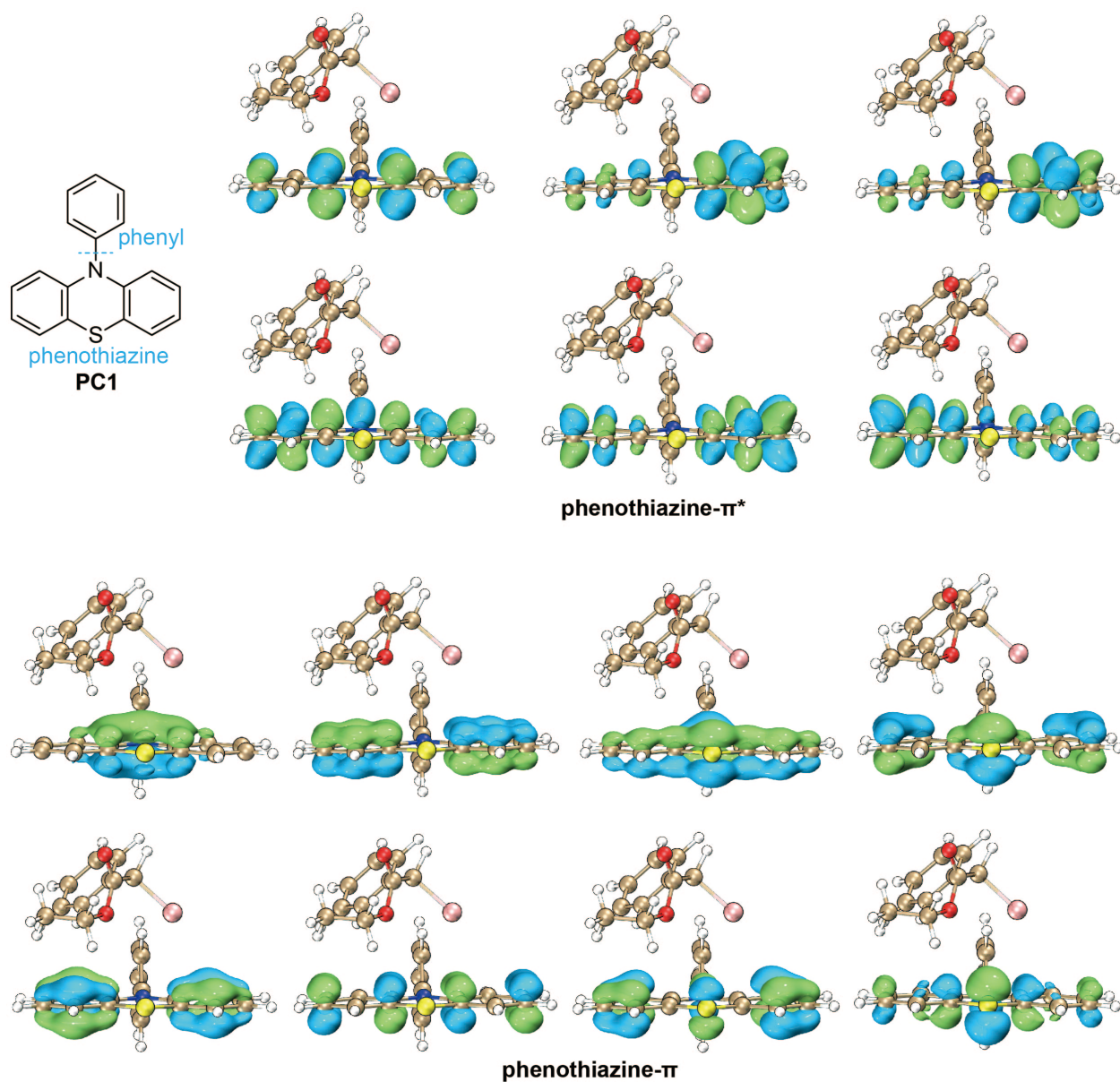


Figure S4: Ground-state (S_0) regional FLMOs corresponding to the fourteen phenothiazine- π/π^* of PC/R-X but at the equilibrium geometry of $^3\text{PC}^*/\text{R-X}$, calculated by PBE0/def2-SVP.

S5. Exciplexes for Activation and Reactivation

From discussions in the main text, it is noticed that the initiator R-X, which can bind with $^1,^3\text{PC}^*$ to form an exciplex $^1,^3\text{PC}^*/\text{R-X}$, becomes a polymer chain $\text{P}_n\text{-X}$ during the polymerization, so that the exciplex becomes $^1,^3\text{PC}^*/\text{P}_n\text{-X}$. The question is then whether $^1,^3\text{PC}^*/\text{R-X}$ and $^1,^3\text{PC}^*/\text{P}_n\text{-X}$ have similar binding strengths $\Delta E_{\text{b}}^{\text{ex}}$. To see this, chemical structures of R-X and $\text{P}_n\text{-X}$ (cf. Fig. S5a) are checked first, which both contain the ethyl- α -bromo-acetate core structure but differ in that the latter has a more bulky α -substituent than the former. Owing to such similarity, R-X and $\text{P}_n\text{-X}$ can bind with the $^3\text{PC}^*$ of PC1 in a similar way (see Fig. S5b and c, respectively) and thus result in $\Delta E_{\text{b}}^{\text{ex}}$ of 11.2 kcal/mol and 11.6 kcal/mol, respectively, which do not differ significantly from each other.

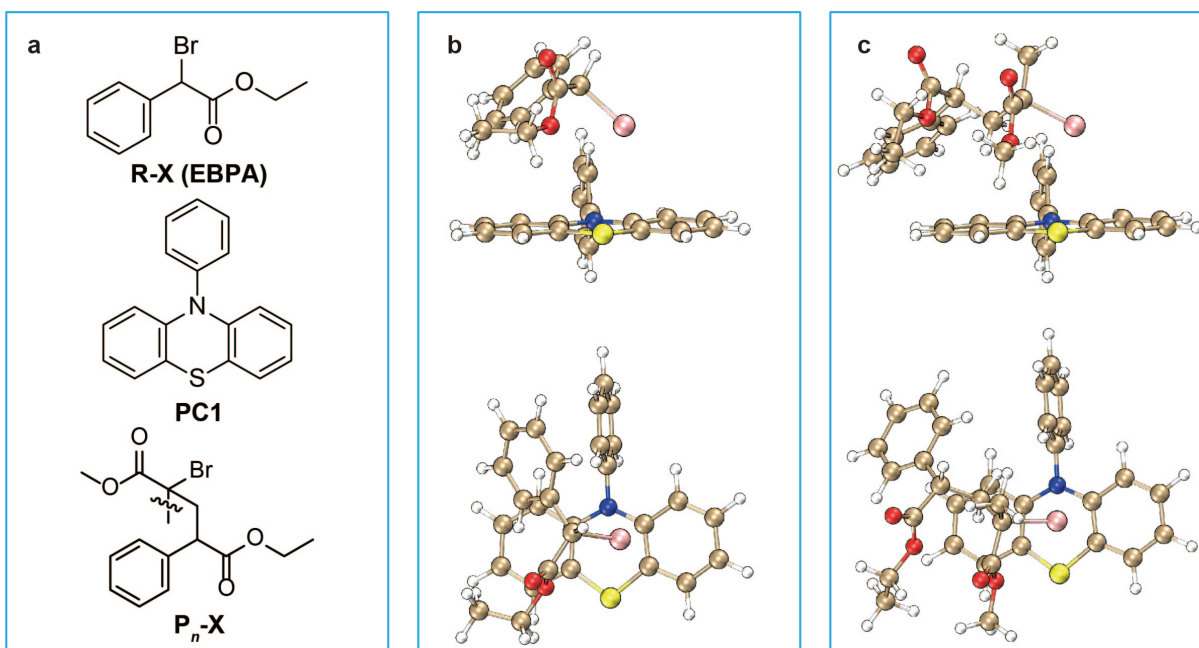


Figure S5: (a) Chemical structures of R-X (EBPA), PC1, and $\text{P}_n\text{-X}$. (b-c) Equilibrium geometries of the exciplexes $^3\text{PC}^*/\text{R-X}$ (b) and $^3\text{PC}^*/\text{P}_n\text{-X}$ (c) for PC1, calculated by UPBE0-D3BJ/def2-SVP/SMD-DMF.

S6. Maximum Initiator Efficiency, Minimum Catalyst Loading and Minimum Molecular weight Dispersity

The ‘maximum initiator efficiency’ (MIE) in O-ATRP is defined as the highest initiator efficiency I^* (best to be $\approx 100\%$) that is possible with a specific PC. On the other hand, the ‘minimum catalyst loading’ (MCL) is defined as the lowest catalyst loading of a PC being sufficient for achieving satisfactory polymerization control (i.e., high I^* and low $\bar{D}$; ideally, $I^* \approx 100\%$ and as low $\bar{D}$ as possible). The ‘minimum molecular weight dispersity’ (MMD) in O-ATRP is defined as the lowest achievable molecular weight dispersity $\bar{D}$ for a particular PC. To determine properly the MIE, MCL and MMD for different PCs, standard O-ATRP conditions are used, where the molar ratio between the monomer and R–X, $[M]:[R-X]$, should be around 100:1~200:1, and monomer conversions should be $\geq 50\%$.

The so-determined MIE for O-ATRP with PC1 (cf. Nos. 1-3 of Table S5), PC4 (cf. Nos. 12-13 of Table S5), and PC5 (cf. Nos. 15-18 of Table S5) turn out to be $\approx 100\%$, whereas the MCL for PC1 (cf. No. 1 of Table S5), PC4 (cf. No. 12 of Table S5), and PC5 (cf. Nos. 17 of Table S5) are 1000 ppm, 50 ppm, and 10 ppm, respectively. As for PC3, it is clear from Nos. 9-11 of Table S5 that the I^* cannot exceed 61% even if the catalyst loading is increased from 0.5 ppm to 100 ppm, indicating an MIE of 61%. Since the best polymerization control with PC3 ($I^* = 61\%$ and $\bar{D} = 1.30$) being achieved at 10 ppm loading (cf. No. 10 of Table S5) is only slightly better than that ($I^* = 53\%$ and $\bar{D} = 1.39$; cf. No. 11 of Table S5) at 0.5 ppm, the MCL for PC3 is then 0.5 ~ 10 ppm. Lastly, as seen in Nos. 4-7 of Table S5, with the loading of PC2 being increased from 1 ppm to 1143 ppm, the I^* is improved from 1% to 14% yet still being very low, meaning that the MCL for PC2 must be $\gg 1000$ ppm. Due to solubility issues, a catalyst loading much higher than 1143 ppm is not possible with PC2, which means that the exact MCL for PC2 cannot be determined. On the other hand, $I^* = 88\%$ (cf. No. 8 in Table S5) is found possible with PC2 by reducing the loading of R–X by nine times (i.e., from $[M]:[R-X] = 875:9$ to $[R-X] = 875:1$), which can be regarded

(in terms of the [R–X]:[PC2] ratio) as increasing the loading of PC2 by nine times. It can then be deduced that the MIE for O-ATRP with PC2 is around 88% and the MCL for PC2 could be up to nine times higher than 1143 nm (i.e., $\gg$ 1000 ppm).

Table S5: Polymerization performances of PC1-5 in O-ATRP.

No.	catalyst	loading ^a	R–X	monomer	[M]:[R–X] ^b	$M_{n,\text{exp}}$ ^c	$M_{n,\text{theo}}$ ^d	I^* ^e	$\bar{D}$ ^f	Ref.
1 ^g	PC1	1000 ppm	EBPA	MMA	100:1	6200	7200	116%	1.30	26
2 ^g	PC1	1000 ppm	EBPA	BMA	100:1	12000	11000	92%	1.25	26
3 ^g	PC1	1000 ppm	EBPA	BMA	100:1	15400	14000	91%	1.32	26
4 ^h	PC2	1143 ppm	EBPA	MMA	875:9	41200	5760	14%	1.29	14
5 ^h	PC2	114 ppm	EBPA	MMA	875:9	125000	6200	5%	1.39	14
6 ^h	PC2	11 ppm	EBPA	MMA	875:9	253000	5200	2%	1.46	14
7 ^h	PC2	1 ppm	EBPA	MMA	875:9	273000	2750	1%	1.57	14
8 ^h	PC2	1143 ppm	EBPA	MMA	875:1	55800	48900	88%	1.65	14
9 ^h	PC3	100 ppm	DBMM	MMA	200:1	17900	10100	56%	1.56	15
10 ^h	PC3	10 ppm	DBMM	MMA	200:1	19300	11800	61%	1.30	15
11 ^h	PC3	0.5 ppm	DBMM	MMA	200:1	23300	12200	53%	1.39	15
12 ^g	PC4	50 ppm	DBMM	MMA	200:1	12200	13900	114%	1.27	16
13 ^g	PC4	25 ppm	DBMM	MMA	200:1	13200	14500	110%	1.58	16
14 ^g	PC4	10 ppm	DBMM	MMA	200:1	14700	11500	78%	1.81	16
15 ^g	PC5	100 ppm	DBMM	MMA	100:1	9500 ^j	10200 ^j	93%	1.09	17
16 ^g	PC5	50 ppm	DBMM	MMA	100:1	7800 ^j	8200 ^j	106%	1.14	17
17 ^g	PC5	10 ppm	DBMM	MMA	100:1	8900 ^j	8200 ^j	92%	1.27	17
18 ^g	PC5	5 ppm	DBMM	MMA	100:1	7400 ^j	7600 ^j	103%	1.42	17

Note: ^aCatalyst loading with respect to the monomer. ^bMolar ratio between the monomer and R–X. ^cExperimentally determined number-averaged molecular weight. ^dTheoretical number-averaged molecular weight derived from monomer conversions. ^eInitiator efficiency, defined as $M_{n,\text{exp}}/M_{n,\text{theo}}$. ^fMolecular weight dispersity, defined as the ratio between the weight-averaged and number-averaged molecular weights. ^gPerformed in DMAc as the solvent. ^hPerformed in DMF as the solvent. ⁱPerformed without an additional solvent (i.e., neat monomers). ^jDerived based on the weight-averaged molecular weight, $\bar{D}$, and I^* . DMAc: N,N-dimethyl acetamide. DMF: N,N-dimethyl formamide. DMSO: dimethyl sulfoxide. EBPA: ethyl- α -bromophenylacetate. DBMM: diethyl 2-bromo-2-methylmalonate. MMA: methyl methacrylate. BMA: benzyl methacrylate. BA: benzyl acrylate.

S7. Potential Side Reaction for $\text{PC}^{\bullet+}$

From discussions in the main text, the unpaired electron in $\text{PC}^{\bullet+}$ resides mainly on S and N, such that a side reaction may occur between S and $\text{P}_n^\cdot$ (NB: N is blocked by phenyl-H and is hence not reactive, see Fig. S6a). To confirm this, the distance between the S of $\text{PC}^{\bullet+}$ and the sp^2 alkyl-C of $\text{P}_n^\cdot$ is shortened from a value of 3.5 Å to the equilibrium (2.0 Å) in a relaxed scan, which does reveal a monotonically decreasing energy profile (see Fig. S6b), so as to lead to an unwanted product $\text{PC}-\text{P}_n^+$.

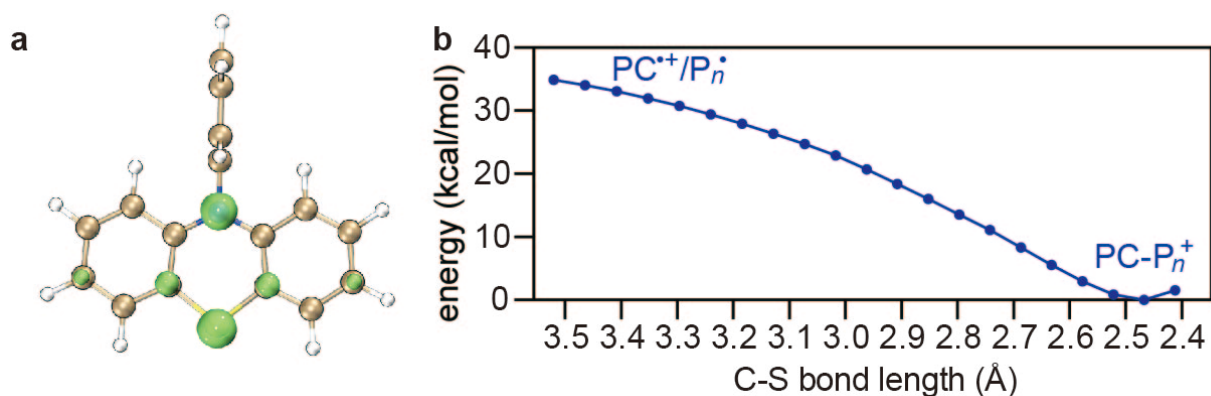


Figure S6: Net Mulliken spin populations of $\text{PC}^{\bullet+}$ (a) as well as relaxed scan of the C–S bond between the sp^2 alkyl-C of $\text{P}_n^\cdot$ and the S of $\text{PC}^{\bullet+}$ (b), using UPBE0-D3BJ/def2-SVP/SMD-DMF.

S8. Validity of New Descriptors for PCs within the Same Family

In the main text, we have examined PCs bear very different chromophore cores and substituents. To broaden the validation scope of our proposed descriptors, we also tested PCs bearing the same chromophore core and similar structures. The most common PC families employed for OQP in O-ATRP encompass dihydrophenazines,^{17,27,28} phenothiazines,²⁹ phenoxazines³⁰ and acridines.³¹ We have selected core-substituted diaryl dihydrophenazines (see Fig. S7) as newly added model systems because these PCs possess following characteristics: (i) similar chemical structures with the same chromophore core; (ii) the ability to mitigate side reactions associated with alkyl core substitution (AkCS) [17-19]; (iii) a wealth of distinguishable experimental results adopting different catalyst loadings, which are ideal for determining the performance descriptors MIE, MCL and MMD. Whereas the reasons for omitting other PC families are as follows: (i) non-core-substituted diaryl dihydrophenazines suffer AkCS effect;^{17,27,28} (ii) non-core-substituted diaryl dihydrophenazines, phenothiazines and phenoxazines are mostly reported with fixed catalyst loadings (e.g. 1000 ppm). The relatively limited experimental data makes it challenging to determine the performance descriptors (MIE, CUD and MMD); (iii) dimethyl acridines, on the other hand, are mostly reported with n-butyl acrylate (BA) as the monomer, making the experimental results less comparable with those adopting methyl methacrylate (MMA).

In the main text, we have identified three performance descriptors (MIE, MCL, and MMD). To gain the MIE, MCL and MMD, the performances for PCs 5-11 are summarized in Table S6. From the experimental data, we can conclude that the MIE for O-ATRP with PC5 (cf. Nos. 1-4 of Table S6), PC6 (cf. Nos. 5-8 of Table S6), PC7 (cf. Nos. 9-10 of Table S6), PC8 (cf. No. 11 of Table S6), PC9 (cf. Nos. 12-15 of Table S6), PC10 (cf. Nos. 16-19 of Table S6), and PC11 (cf. No. 20 of Table S6) turn out to be $\approx 100\%$. The MCL for PC5 (cf. Nos. 1-4 of Table S6), PC6 (cf. Nos. 5-8 of Table S6), PC9 (cf. Nos. 12-15 of Table

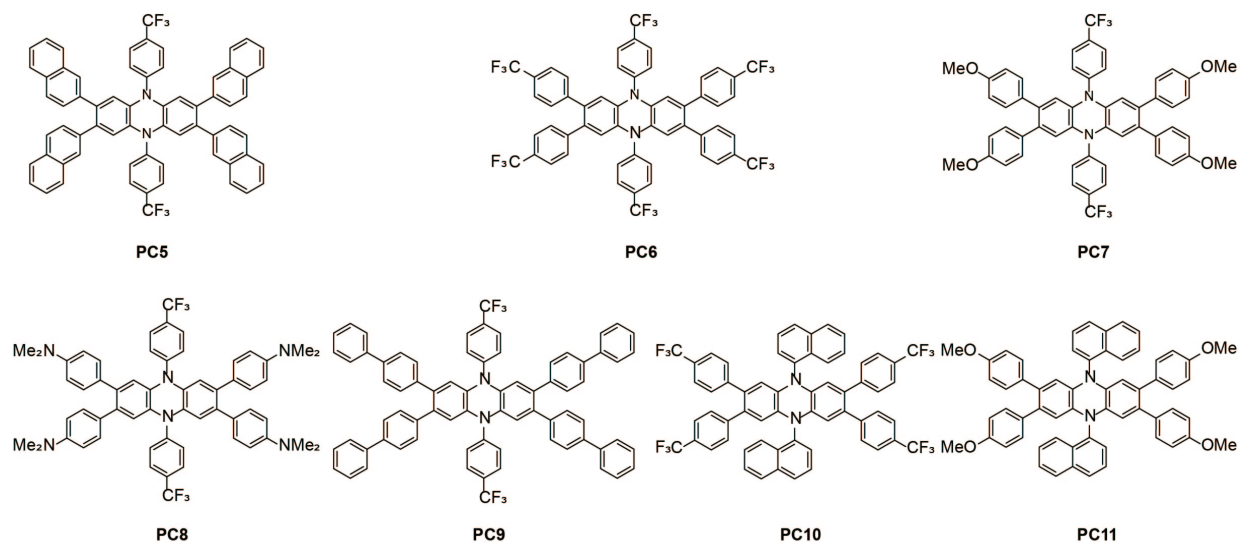


Figure S7: Chemical structures of core-substituted diaryl dihydrophenazines (PC5-11)

S6), PC10 (cf. Nos. 16-19 of Table S6) are around 50 ppm, whereas for PC7 (cf. Nos. 9-10 of Table S6), PC8 (cf. No. 11 of Table S6), and PC11 (cf. No. 20 of Table S6), it is hard to give precise MCLs for lacking of more detailed controlled experiments. However, based on the existing experimental data,^{17,28} we can conclude qualitatively that the MCLs are higher than 100 ppm. The MMD for PC7 (cf. Nos. 9-10 of Table S6), PC8 (cf. No. 11 of Table S6), and PC11 (cf. No. 20 of Table S6) are higher than that for PC5 (cf. Nos. 1-4 of Table S6), PC6 (cf. Nos. 5-8 of Table S6), PC9 (cf. Nos. 12-15 of Table S6) and PC10 (cf. Nos. 16-19 of Table S6), indicating less control for polymerization.

In the main text, we have identified three pairs of property-performance descriptors (AED-MIE, CUD-MCL, and DED-MMD). To validate these descriptors pairs, we have included corresponding results for PCs 5-11 in Table S7. By carefully analyzing these results, the following conclusions can be drawn: (i) Generally, the property descriptors all well align with relevant performance descriptors in the expected manner. (ii) Specifically, the AED values for PC5-11 are all exceeded than that PC3 at a value of 9.6×10^1 . This implies a more rapid conversion of R-X initiators to polymer chains, thereby rendering a higher MIE. This observation aligns perfectly with the reported MIE values, wherein PC5-11 yield a MIE of approximately to 100%, higher than that PC3 at a value of 61%. (iii) A lower MCL

Table S6: Polymerization performances of PCs 5-11 in O-ATRP.

No.	catalyst	loading ^a	R–X	monomer	[M]:[R–X] ^b	$M_{n,exp}$ ^c	$M_{n,theo}$ ^d	I^*e	$\bar{D}^f$	Ref.
1 ^g	PC5	100 ppm	DBMM	MMA	100:1	9500 ^j	10200 ^j	93%	1.09	17
2 ^g	PC5	50 ppm	DBMM	MMA	100:1	7800 ^j	8200 ^j	106%	1.14	17
3 ^g	PC5	10 ppm	DBMM	MMA	100:1	8900 ^j	8200 ^j	92%	1.27	17
4 ^g	PC5	5 ppm	DBMM	MMA	100:1	7400 ^j	7600 ^j	103%	1.42	17
5 ^g	PC6	500 ppm	DBMM	MMA	100:1	7180 ^j	7010 ^j	98%	1.18	17
6 ^g	PC6	100 ppm	DBMM	MMA	100:1	7720 ^j	7640 ^j	99%	1.14	17
7 ^g	PC6	50 ppm	DBMM	MMA	100:1	9560 ^j	9040 ^j	95%	1.14	17
8 ^g	PC6	10 ppm	DBMM	MMA	100:1	8000 ^j	7620 ^j	95%	1.50	17
9 ^g	PC7	1000 ppm	DBMM	MMA	100:1	4500 ^j	4730 ^j	105%	1.34	17
10 ^g	PC7	100 ppm	DBMM	MMA	100:1	8520 ^j	7960 ^j	93%	1.49	17
11 ^g	PC8	1000 ppm	DBMM	MMA	100:1	7470 ^j	9640 ^j	129%	1.82	17
12 ^g	PC9	500 ppm	DBMM	MMA	100:1	6900 ^j	8140 ^j	118%	1.12	17
13 ^g	PC9	100 ppm	DBMM	MMA	100:1	6620 ^j	6480 ^j	98%	1.13	17
14 ^g	PC9	50 ppm	DBMM	MMA	100:1	8940 ^j	9560 ^j	107%	1.13	17
15 ^g	PC9	10 ppm	DBMM	MMA	100:1	7830 ^j	7550 ^j	96%	1.29	17
16 ^g	PC10	500 ppm	DBMM	MMA	100:1	7530 ^j	7030 ^j	93%	1.07	28
17 ^g	PC10	100 ppm	DBMM	MMA	100:1	7710 ^j	6710 ^j	87%	1.16	28
18 ^g	PC10	50 ppm	DBMM	MMA	100:1	8800 ^j	8090 ^j	92%	1.07	28
19 ^g	PC10	10 ppm	DBMM	MMA	100:1	7170 ^j	6940 ^j	97%	1.49	28
20 ^g	PC11	1000 ppm	DBMM	MMA	100:1	5320 ^j	5370 ^j	101%	1.57	28

Note: ^aCatalyst loading with respect to the monomer. ^bMolar ratio between the monomer and R–X. ^cExperimentally determined number-averaged molecular weight. ^dTheoretical number-averaged molecular weight derived from monomer conversions. ^eInitiator efficiency, defined as $M_{n,exp}/M_{n,theo}$. ^fMolecular weight dispersity, defined as the ratio between the weight-averaged and number-averaged molecular weights. ^gPerformed in DMAc as the solvent. DMAc: N,N-dimethyl acetamide. DBMM: diethyl 2-bromo-2-methylmalonate. MMA: methyl methacrylate.

must be achieved with a higher CUD. Indeed, the MCL values for PC7, PC8 and PC11 with lower CUD values are higher than those for PC5, PC6, PC9 and PC10 with high CUD values. Thus, the CUD results exhibit a strong correlation with MCL for PC5-11. (vi) When comparing the DED values, it becomes apparent that when the DED is sufficiently low (as seen in PC7, PC8 and PC11), the MMD will tends to be significantly high, signifying a less efficient alternating growth of polymer chains. Thus, the DED values align well with MMD.

In short, the newly added PC6-11 of the core-substituted diaryl dihydrophenazines also well verify the validity of the three pairs of property-performance descriptors established in this work.

Table S7: Performances of catalysts in O-ATRP and calculated molecular descriptors

No.	catalyst	polymerisation ^a		descriptor ^b										DED
		loading ppm	I^{*c}	D	ΔE^{ex} kcal/mol	$\tau_{\text{ns}}^{\text{ex}}$ ns	$\Delta E^\ddagger$ kcal/mol	$\tau^\ddagger$ ns	$\Delta E^{\text{PC-X}}$ kcal/mol	$\tau_{\text{ns}}^{\text{PC-X}}$ ns	$\Delta E_{\text{de}}^\ddagger$ kcal/mol	$\tau_{\text{ns}}^{\ddagger_{\text{de}}}$ ns	CUD ns^2	
5a	PC5 ¹⁷	50	106%	1.14	17.5	7.6×10^8	3.3	2.9×10^{-2}	17.4	6.3×10^8	3.9	8.5×10^{-2}	2.6×10^{10}	3.1×10^{-1}
5b		10	92%	1.27										
6a		50	95%	1.14	17.4	6.5×10^8	4.3	1.6×10^{-1}	18.2	2.5×10^9	3.8	6.8×10^{-2}	4.1×10^9	1.6×10^{18}
6b	PC6 ¹⁷	10	95%	1.50										
7a		1000	105%	1.34	17.2	4.6×10^8	1.5	1.4×10^{-3}	16.8	2.3×10^8	4.6	2.6×10^{-1}	3.3×10^{11}	2.7×10^{-3}
7b		100	93%	1.49	17.1	3.9×10^8	0.9	5.1×10^{-4}	15.7	3.7×10^7	5.4	1.0×10^0	7.6×10^{11}	4.7×10^{-5}
8	PC8 ¹⁷	1000	129%	1.82	17.1									
9a		50	107%	1.13	17.4	6.5×10^8	3.0	1.8×10^{-2}	17.4	6.5×10^8	4.3	1.6×10^{-1}	3.7×10^{10}	1.1×10^{-1}
9b		10	96%	1.29										
10a	PC10 ²⁷	50	92%	1.07										
10b		10	97%	1.49	17.4	6.5×10^8	3.1	2.1×10^{-2}	18.0	1.6×10^9	4.1	1.1×10^{-1}	3.1×10^{10}	5.1×10^{-1}
11		1000	101%	1.57	16.6	1.7×10^8	1.1	7.2×10^{-4}	16.6	1.7×10^8	5.0	5.2×10^{-1}	2.3×10^{11}	1.4×10^{-3}

Note: ^aResults with diethyl-2-bromo-2-methylmalonate initiator solvated in DMAc, methyl methacrylates as the monomer, and a formulation of [monomer]:[initiator] = 100:1. ^b $\Delta E^\ddagger$ calculated with (LOSC-) PBE0-D3BJ/def2-SVP/SMD-DMF for PC5-11; ΔE_b^{ex} , $\Delta E_b^{\text{PC-X}}$ and $\Delta E_{\text{de}}^\ddagger$ calculated with UPBE0-D3BJ/def2-SVP/SMD-DMF for PC5-11. ^cthe value of $I^* \gg 100\%$ indicates autoinitiation or the occurrence of other side reactions.

Supplementary Appendix A: Minimum Energy Crossing Point

The geometry for the minimum energy crossing point between S_1 and T_2 of PC5 is optimized by PBE0-D3BJ/def2-SVP, at which the spin orbit coupling matrix element between S_1 and T_2 is calculated by sf-X2C-TDDFT-SOC³²/PBE0-D3BJ/X2C-SVPall using the BDF^{24,25} software package.

Coordinates (Å):

C, 1.89326648, -2.92199012, 0.94192309
C, 2.19103626, -1.63655047, 0.48655190
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C, -0.08540284, -1.31534896, -0.30174600
C, -0.39988529, -2.58736336, 0.20857547
C, 0.54109175, -3.38240771, 0.85808881
C, -0.71036307, 0.72349886, -1.41353227
C, 0.59166545, 1.24635132, -1.19740592
C, 0.87701415, 2.55328704, -1.61145627
C, -0.06354454, 3.34947757, -2.26535405
C, -1.33730297, 2.78296810, -2.58632992
C, -1.63958602, 1.50496651, -2.12173655
N, -1.01969868, -0.53726378, -0.95030163
C, -2.33277843, -1.04578022, -1.14603979
C, -3.35680136, -0.71503052, -0.22911650
C, -2.60987977, -1.87470374, -2.25613281
C, -4.62341404, -1.20189323, -0.42225242
C, -3.87762830, -2.36039489, -2.44176341
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H, -2.60568462, 1.06510468, -2.36535142
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C, 5.40067637, 1.98242072, 0.05083606
H, 5.81925730, 1.31725041, -1.95813637
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F, -6.63327196, -3.39805779, -0.70768981
F, -6.44063329, -3.23496972, -2.85356823
F, -7.20277861, -1.57289099, -1.69894124
F, 6.77522930, 3.64559355, 0.96911409
F, 7.45971908, 2.68447858, -0.83860984
F, 7.49959505, 1.62169536, 1.03454625

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C, 4.20809652, -7.31008333, 1.34055746
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C, 6.24001386, -6.13647744, 2.87307562
C, 5.24757670, -8.07432805, 1.81637624
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H, 2.99054335, 6.62188138, -3.55224380
C, 1.35766101, 8.79578000, -3.39992345
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H, -2.26346736, 7.92862268, -2.25586842
C, 0.41333469, 9.78882360, -3.27850731
H, 2.37383453, 9.03270887, -3.72478085
H, -1.64450436, 10.27117796, -2.77166011
H, 0.67504387, 10.82534019, -3.50658862

Supplementary Appendix B: Molecular Coordinates (Å)

³PC*/R–X for PC1

charge = 0, multiplicity = 3

C, 2.68357125431424, -3.01384809840874, -0.02662753706230
C, 3.05782291581401, -1.75563995905385, -0.42872158320506
C, 2.15049219764131, -0.89517711908349, -1.09302075984551
C, 0.78722963298383, -1.33703102653332, -1.34160642704566
C, 0.44209643303819, -2.64509927659099, -0.91908209549569
C, 1.34581797498276, -3.46746571311319, -0.28555629631126
C, 0.09495291349491, 0.74552228137746, -2.45368411879028
C, 1.39670712270711, 1.37953531186588, -2.34541646689906
C, 1.58790858729017, 2.68538063436542, -2.85879801532758
C, 0.56299448344910, 3.37122260486772, -3.46137591771402
C, -0.72782712654371, 2.75744983623952, -3.56648628892950
C, -0.94030391416158, 1.49077562027187, -3.07270079225040
S, 2.72273980346414, 0.64244017400612, -1.56232088126760
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C, -2.38316965757591, -0.80124645624959, -1.04793627249957
C, -1.83541504437593, -1.74615051914611, -3.21719034756374
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H, 0.73084235858892, 4.37638383340220, -3.85373607816358
H, -1.55286122584002, 3.29523436885425, -4.03830840965880
H, -1.93191525975938, 1.04604356022255, -3.15960206306750
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H, -5.07091901913852, -2.41368429398847, -2.38407340677507
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C, -2.76997301772554, -2.30711426815658, 2.39721522515116
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H, -0.96606583042779, -3.37999326861375, 1.88096265071444
H, -3.40604696828393, -3.19494856412826, 2.35787318322795
C, -0.30045209398920, 1.21531057343173, 2.53615746689618
H, -0.80494036172448, 1.98331816898919, 3.13281130306513
Br, -0.13973670770213, 1.99536014058518, 0.73458446918963
C, 1.06271887352897, 0.99953027811026, 3.16823762609596
O, 1.25827575535013, 1.24431309825698, 4.33245457955355
O, 1.95706833588136, 0.49585249876649, 2.33586613283603

C, 3.25487476524913, 0.17597061971870, 2.85859445305387
C, 3.27529170213719, -1.19494161577685, 3.48605870044191
H, 3.54627370909822, 0.95305355825110, 3.58010226682562
H, 3.92489332018821, 0.23230011718968, 1.99046253106111
H, 2.58978712786486, -1.25080743194812, 4.34468050743151
H, 2.99682267562312, -1.97029096578776, 2.75644744045543
H, 4.29158117565105, -1.41576357575110, 3.84692978809273

¹PC*/R–X for PC2

charge = 0, multiplicity = 1

C, -3.01740592364594, 1.05335183949919, 0.88968861262040
C, -1.77785725333103, 0.42222369124150, 0.58292549673453
C, -0.87956687608174, 1.07110863374438, -0.31560260529844
C, -1.23628223771038, 2.34363155472241, -0.87460773989223
C, -2.47763474777827, 2.93008727639139, -0.53330378466393
C, -3.35169654406483, 2.28201443044501, 0.33913121739561
H, -3.71957622730170, 0.57528307657879, 1.57225305117185
C, 0.38038224570482, 0.48846386747463, -0.64658063006699
C, -0.33479174585600, 2.99714447545067, -1.74688219305065
H, -2.73800972309807, 3.90081907828531, -0.96348941925553
H, -4.30802061675174, 2.74553043223954, 0.59431791037124
C, 0.89030732780903, 2.41355481784519, -2.06983063656324
C, 1.24664495479651, 1.18498847339262, -1.53619391165737
H, -0.61514804465502, 3.96863444217599, -2.16258052383676
H, 1.57915138380882, 2.92993907302476, -2.74298245606174
H, 2.21620131184729, 0.76283417441040, -1.79407450755784
C, -1.39840019992147, -0.83075517510460, 1.17942603827254

C, -0.13034237102185, -1.40299689761984, 0.86406463802381
C, -2.24500610896132, -1.50624931942026, 2.10444157558772
C, 0.75840946629320, -0.76524480873485, -0.05200072628190
C, 0.27027565937404, -2.62628515642436, 1.49897808039527
C, -1.84925851511025, -2.69246219141829, 2.70506411265857
H, -3.22041945974005, -1.09047437535946, 2.35476705462378
C, 2.01586585275341, -1.37384222193166, -0.32597271517259
C, 1.53882638694028, -3.17873300535239, 1.20588325444242
C, -0.60603991935542, -3.25396908303239, 2.41571187160940
H, -2.51817676423656, -3.18800250242146, 3.41324236319139
C, 2.39369734426671, -2.55231282947637, 0.29814212346340
H, 2.71043156634532, -0.90377229263532, -1.01997046584706
H, 1.83636617634036, -4.10672769046363, 1.70145490880075
H, -0.29025130948279, -4.18493310177295, 2.89393626446930
H, 3.37057854338408, -2.99025383316805, 0.07823499888195
C, 4.42240530218232, 1.04721446313272, 1.70582706204991
Br 4.93098980276769, 1.11225750415020, -0.17664773936620
C 5.33985565546669, 1.95695927660508, 2.51298519877480
O 5.86342074499541, 2.96240455259945, 2.11342743158250
O 5.41144723285877, 1.49593483541894, 3.75514710496522
C 6.06967022757024, 2.32045253607759, 4.73120801990403
C 5.12849709717677, 3.36780423922899, 5.27591283536860
H 6.95696897312639, 2.77622266869578, 4.26879369421990
H 6.39376778681579, 1.62153328603963, 5.51338958827768
H 4.81947900720854, 4.06877355687367, 4.48635429831424
H 4.23027676258387, 2.90071890529325, 5.70696716621628
H 5.63397961372516, 3.94232580697882, 6.06653725147173

C 2.99568572417430, 1.46127336629264, 1.94993412151487
C 2.52028686153673, 2.70639275557723, 1.51859170809077
C 2.16011519121587, 0.62521392687636, 2.69622479437897
C 1.21951432527157, 3.10086951980761, 1.82079329416551
H 3.17256215227376, 3.36090034961134, 0.93477120255712
C 0.85963069315460, 1.02579352859494, 3.00449105815591
H 2.53009164318614, -0.34759723816270, 3.03073639503492
C 0.38633520967280, 2.26094120605054, 2.56470530663509
H 0.84996951827602, 4.06725898930323, 1.46904702873826
H 0.20909388457695, 0.36001007548694, 3.57661460112675
H -0.63844557485688, 2.56645499459286, 2.79038633926231
H 4.57083853348081, 0.00868504228879, 2.02469898105283

³PC*/R–X for PC3

charge = 0, multiplicity = 3

C, -0.46803507337705, -3.59217977846356, 0.88347930119004
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C, -0.97665872518221, -2.72048273126062, 1.85733699799334
C, 0.31639183320698, -4.68192863615043, 1.28098881653883
C, -1.41590433622402, -3.94661164740954, -2.72412176498861
C, -1.81533588528161, -5.46859801890506, -0.89104803330024
C, -0.68406993606819, -2.92442030867243, 3.20346688731802
H, -1.59649106820182, -1.87443042352153, 1.55227554470404
C, 0.60001672953192, -4.88207869569511, 2.63041941264447
C, -2.00169671125538, -4.85450937779686, -3.59996183395299
H, -1.04976106490773, -2.99070397120921, -3.10059655737099
C, -2.39170156208047, -6.37100963007001, -1.78070863987409

C, 0.11001597244099, -4.00266089042799, 3.59690909259542
H, -1.08517204763075, -2.23515470926828, 3.95116836149329
H, 1.22200125234850, -5.73086361775457, 2.92641098576008
C, -2.48724780375509, -6.07971729274182, -3.14208216094305
H, -2.07558719698777, -4.59527882326708, -4.65956811109936
H, -2.78103811926254, -7.31688902561982, -1.39434558159798
H, 0.34247447462542, -4.15969649352903, 4.65293701438671
H, -2.94187674491987, -6.79271658980316, -3.83366514635417
C, -0.51335297940421, -1.97889653638950, -0.88896894848221
C, 0.77294238322275, -1.42939752409561, -0.93468320919089
C, -1.64504008309816, -1.09725053077928, -1.07354685953501
C, 0.98603419212863, -0.03943135108458, -1.11227319476192
C, -1.45147217857483, 0.30359611130943, -1.14419166459367
C, -0.16392257640647, 0.84916922583181, -1.10751373203181
N, -0.70732175784639, -3.32051632449230, -0.48892570693496
C, 0.00526724030796, 2.24776103824730, -1.10428880284172
N, 0.15398771937734, 3.40538806557317, -1.09238077227542
C, -2.94963932503399, -1.62824728865707, -1.12626708442696
N, -4.02439521844270, -2.08246281652460, -1.15760838826940
N, 2.24525213766739, 0.39811423902009, -1.57370096630597
C, 2.62850821554476, -0.04058975434512, -2.86487062600491
C, 2.97332161746911, 1.34961447858636, -0.86222233448121
C, 1.67532016830694, -0.04183779924302, -3.89437149025560
C, 3.92388396978113, -0.51180734902316, -3.11926310732925
C, 2.69093090241381, 1.55330934586024, 0.50117820902182
C, 3.97217014101556, 2.13274816307075, -1.47304038136506
C, 2.01377681662358, -0.51966684920809, -5.15712111739281

H, 0.66977513850131, 0.33633495882896, -3.69763694608815
C, 4.25169596026785, -0.98651245345353, -4.38608091499841
C, 3.41266034960348, 2.48216283281325, 1.23945551936001
H, 1.89848960460036, 0.97601901826544, 0.97610226622376
C, 4.68697838096480, 3.05701576614443, -0.72137334992597
C, 3.30091133549009, -0.99709079468299, -5.40860018884504
H, 1.26324552282809, -0.51469760539892, -5.95147609866868
H, 5.26085728052761, -1.36258576525479, -4.57205190780631
C, 4.42203768068794, 3.23627764576929, 0.63938480682356
H, 3.18802109564892, 2.61167694672241, 2.30121220333914
H, 5.45878286765092, 3.65614684498297, -1.21122318147130
H, 3.56366097676911, -1.37564918126599, -6.39921726286174
H, 4.98965925573609, 3.96501897680672, 1.22240120072964
N, 1.91039260405790, -2.23887318293015, -0.76349590058701
C, 2.82157492668157, -1.91743126151242, 0.26315861942258
C, 2.10717330523645, -3.37859459356439, -1.54999151652066
C, 2.32986040844579, -1.49739890312896, 1.50748611732286
C, 4.20536829166161, -2.04318755255382, 0.06012466710974
C, 1.68731132352691, -3.37605896754525, -2.89088842555674
C, 2.75669329851647, -4.51124538924096, -1.02213305377758
C, 3.21633955267862, -1.21335334132797, 2.54109746971098
H, 1.25230152664382, -1.43530647686762, 1.66303100491378
C, 5.07950221534380, -1.74102153715859, 1.09589192252075
C, 1.91561792569210, -4.48901338809170, -3.68976443616190
H, 1.21507409950014, -2.48651088496879, -3.30572515058383
C, 2.97245256798944, -5.61713799208021, -1.83073806818817
C, 4.59095755604245, -1.32889753449534, 2.33959170308969

H, 2.82803271655354, -0.90362677891547, 3.51385814131448
H, 6.15610371791210, -1.82461373274643, 0.93024636820169
C, 2.55534699581967, -5.61308681553013, -3.16635001472565
H, 1.59483276946217, -4.47277236137398, -4.73375366826077
H, 3.46386817699488, -6.49884278288087, -1.41304211919140
H, 5.28515137703237, -1.10083053813215, 3.15165236216673
H, 2.73128861439186, -6.48772819138401, -3.79678768643911
H, 4.66761173374206, -0.51129883068492, -2.32120825829296
H, 4.17980304008227, 2.02479699105526, -2.53816547408719
H, 3.06777921086298, -4.52389266177542, 0.02287181764121
H, 4.58674387978075, -2.36587730560209, -0.90939036502491
H, -1.77303689148481, -5.71589793931257, 0.17008456478941
H, 0.70946174928893, -5.36758215866455, 0.52921504282132
N, -2.56995788397383, 1.15246204838047, -1.25363372055124
C, -3.54109909148445, 1.13007786657007, -0.23371811109526
C, -2.66157049973326, 2.00040264492344, -2.37752116244619
C, -3.14788988651000, 0.84116843021916, 1.08100926904669
C, -4.89432513671633, 1.37405523079931, -0.50569356432387
C, -2.18921624265628, 1.55152114411608, -3.61906090446591
C, -3.18487662709612, 3.29585660545312, -2.26974301001884
C, -4.09183794065166, 0.78997300477729, 2.10205313606762
H, -2.09316212154475, 0.67208998214684, 1.30508707691152
C, -5.82680098111575, 1.34569675365085, 0.52776455534601
H, -5.21731311937964, 1.57946423634184, -1.52779101189748
C, -2.22605621997584, 2.39333033621595, -4.72778664270200
H, -1.79322423335428, 0.53744142107600, -3.71208698899877
C, -3.23660619108203, 4.12162881864130, -3.38877697026398

H, -3.53900236286577, 3.65646966916095, -1.30306560665464
C, -5.43647853256736, 1.04993924783314, 1.83543592116289
H, -3.76355418910899, 0.56616982102356, 3.12033282075841
H, -6.87809031311811, 1.54225543240528, 0.30168427151903
C, -2.75358131767413, 3.68062929602633, -4.62225518858268
H, -1.84879236085899, 2.03028761379462, -5.68734580237319
H, -3.64460176602723, 5.13077805461811, -3.28844305863004
H, -6.17534355641266, 1.02410291298910, 2.63978260374049
H, -2.78759917437110, 4.33710458957134, -5.49493128099900
C, -3.56076552058422, 4.53893160355368, 1.52629726956238
C, -2.23480062472891, 4.10820186353995, 1.47403232494857
C, -1.59844145590353, 3.65049066579756, 2.63242858663387
C, -2.29989031459410, 3.63420168415222, 3.84512266895438
C, -3.62449251180177, 4.05817995375268, 3.89181685156487
C, -4.25897995487877, 4.51003301590307, 2.73198506632355
H, -4.05199907039669, 4.89339113858240, 0.61665000169520
H, -1.68658587919294, 4.12206328610797, 0.52866367672655
H, -1.80747653201524, 3.27420456828934, 4.75128653161446
H, -4.16800436092671, 4.03357503330365, 4.83962987385774
H, -5.30089405794775, 4.83776875225353, 2.77013380431973
C, -0.16142615907410, 3.21388172422485, 2.55432709920940
H, 0.18641614658619, 3.23588651726837, 1.51521772746143
Br, 0.06233149048121, 1.35145289172746, 3.15115876512805
C, 0.73516031773304, 4.15707915095086, 3.33796244277943
O, 1.29689858256436, 5.07577458632123, 2.79666949937296
O, 0.76793515393733, 3.89830171530791, 4.63331452470744
C, 1.47928035142392, 4.81702265988896, 5.47893558117190

C, 0.60751944510465, 5.98210142527912, 5.87319295025498
H, 2.38744487147336, 5.14907869011828, 4.95564232741246
H, 1.77348834527879, 4.21999746267111, 6.35239326930942
H, 0.32103678680068, 6.58135654794980, 4.99616952738584
H, -0.30674771284845, 5.63910252854716, 6.38087880049552
H, 1.15967822614859, 6.63508443362576, 6.56620078161185

³PC*/R–X for PC4

charge = 0, multiplicity = 3

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C, 3.81415260912668, 1.70337835107665, -0.01484146139370
C, 3.48657155324312, 2.05097230468051, 2.72921734190611
C, 2.41936884256555, 2.36537572494061, 1.86635704941984
C, 2.62944237724569, 2.22999978813316, 0.47976534129145
C, 1.10510726787374, 2.70430877688264, 2.43009078422934
H, 3.34559128804638, 2.18111672204847, 3.80356156772851
H, 5.45855566193241, 1.18767291733321, 2.91937044875113
N, 5.93941830821706, 0.55360836671496, 0.37783581255833
H, 1.84417374764887, 2.51902915119089, -0.22200264843136
H, 3.95266586289283, 1.56500060315982, -1.08992675578789
C, -0.05481123872508, 2.40809040012950, 1.73428285817498
N, 1.05574570614681, 3.16024311996141, 3.71938896910355
C, -0.16286079948198, 3.28204837777294, 4.25541519976575
N, -1.31913412976082, 2.96966415405643, 3.69197824178952
C, -1.29679086362510, 2.50488531313953, 2.39887863984569
H, 0.00498877841374, 1.99104363601943, 0.72983738346786

C, -2.51239420807353, 1.98689255879220, 1.82473606827511
 C, -0.21808394041565, 3.79020253175562, 5.65887690376883
 C, -2.61411218600829, 1.62225109340184, 0.45206950624059
 C, -3.73027005027408, 0.97773349251684, -0.04397055605704
 C, -3.64827353407513, 1.73287598755159, 2.64488167835733
 C, -4.76075236685845, 1.07157213240136, 2.15440659856707
 C, -4.79949933455397, 0.67270555682099, 0.81158529434915
 H, -1.79636612385646, 1.84367004790896, -0.23569325256593
 H, -3.78148656668112, 0.68792061344498, -1.09639502472657
 H, -3.60632599114185, 2.02318569498092, 3.69575450263790
 H, -5.60224928481906, 0.83718381905731, 2.81145759282949
 C, 0.95991898198409, 4.12008441690690, 6.34355360958460
 C, 0.91246910660006, 4.58410984889364, 7.65679867626109
 C, -0.31413045459473, 4.72721573568511, 8.30695421906592
 C, -1.49342455563034, 4.40485400728750, 7.63201477508807
 C, -1.44532732764160, 3.94121378029950, 6.31948920498263
 H, -2.36139296759389, 3.68965686987350, 5.78224228267113
 H, -2.45864479541831, 4.51674999126535, 8.13334373219623
 H, 1.91274720849123, 4.00618498863437, 5.82369992743381
 H, 1.84037861976954, 4.83612992093479, 8.17738853441180
 H, -0.35180933252703, 5.09060008193692, 9.33738198162324
 N, -5.89599381895769, -0.11251525392302, 0.32301203672805
 C, -7.08393706857083, 0.50511120950215, -0.00139701042520
 C, -5.71324056266465, -1.47433836658536, 0.18178572547907
 C, -6.75461529576261, -2.30094030658410, -0.30504936527413
 C, -8.19103978878405, -0.24832404672445, -0.46331861852286
 C, -8.12895286759742, -1.75410706847617, -0.64608083343161

C, -7.19384083434323, 1.91031506633719, 0.11759901097485
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 C, -9.50200722177024, 1.82579341302513, -0.62765121248376
 C, -9.36483605338265, 0.43152664993150, -0.75734607785985
 C, -4.46888833558988, -2.05083950518588, 0.53016962434597
 C, -4.24764909406750, -3.39784505893636, 0.36448093799814
 C, -5.25590631125017, -4.24318708626524, -0.14751022708249
 C, -6.49711677292627, -3.65799081505140, -0.45457680361164
 C, -9.16244377155144, -2.41435028125516, 0.28834063564145
 H, -10.17657395789445, -2.05659568166816, 0.05811581611890
 H, -9.15293125211110, -3.50686226568396, 0.16247784389610
 H, -8.94345738137389, -2.18415139921616, 1.34167002805328
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 H, -10.22624570943706, -0.15017837636907, -1.08651455498560
 H, -3.67739392648220, -1.42184732211078, 0.93467837626682
 H, -3.28072002017539, -3.81008710750247, 0.65715223259414
 H, -7.29045232978453, -4.29197424784977, -0.85239438096868
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 C, -3.70562314422178, -6.16374775487596, -0.53174209709494
 C, -3.44580972367698, -7.51444382708604, -0.72912174400911
 C, -4.50679082440694, -8.43230111760281, -0.73961776294483
 C, -6.06348067856077, -6.61406482280638, -0.37248227156393

C, -5.82007242920778, -7.96258764219837, -0.55899100037442
O, -4.36127457036266, -9.75054203332918, -0.91225163747628
C, -3.06420443691863, -10.27750526150736, -1.08175235243067
H, -2.86442973743920, -5.46846756285321, -0.54793687448743
H, -2.41672452336879, -7.84248821902306, -0.87899604905683
H, -7.09324900841336, -6.28609280394991, -0.21523691978470
H, -6.63890149424284, -8.68531549377181, -0.55984865272511
C, -10.76445325616504, 2.49914542786837, -0.95134878268327
C, -11.07310191612513, 3.76503109954757, -0.42276612181667
C, -12.26752581316915, 4.41296562296675, -0.71394726576271
C, -13.20142582030245, 3.80366085194922, -1.56550758220911
C, -12.90905806631310, 2.53968135378999, -2.10821569984151
C, -11.72012603609290, 1.90409563622814, -1.80324193498747
H, -13.63604875700830, 2.07713917770519, -2.77929437347732
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H, -10.37583918672195, 4.25648350375766, 0.25872037006754
H, -12.46691280501122, 5.38830145502146, -0.26905801530968
O, -14.37503845317538, 4.34376511546272, -1.90956322269934
C, -14.72026542543393, 5.61369235168766, -1.40242480220041
C, 5.78262455861007, -0.81782683496100, 0.18762168467567
C, 6.86701148423722, -1.63083366063597, -0.19564199747937
C, 8.27638376805649, -1.07317550439984, -0.38017153219127
C, 7.14565614915682, 1.18840008236206, 0.11208415238204
C, 8.28262986167694, 0.45096181247242, -0.27573003860989
C, 7.24173023321581, 2.58755663032068, 0.22319526071997
C, 8.43302074300353, 3.24722773460352, -0.03462387630674
C, 9.46680950714994, 1.14732026210626, -0.52373942697854

C, 9.58343098984287, 2.53996792591756, -0.41566702676246
H, 6.35962205799742, 3.16310553492209, 0.50702421611926
H, 8.45689057370051, 4.33680745453719, 0.04243468148564
H, 10.35531492018161, 0.57034042677525, -0.78865441336507
C, 8.81691017787313, -1.49451346236668, -1.75710146015819
H, 8.18605152643040, -1.09614745916708, -2.56648008506237
H, 8.84646903391624, -2.58982398293382, -1.85279511267296
H, 9.84267880882703, -1.12826755547276, -1.90987161811600
C, 9.18360870803083, -1.64758648323132, 0.72331439556013
H, 8.81782137969334, -1.36105838462070, 1.72132839079078
H, 10.21450049173363, -1.27608709588719, 0.61595770688827
H, 9.21354291775235, -2.74702072300145, 0.67216317658738
C, 4.52292403670678, -1.41467225276850, 0.38200741933084
C, 4.33281033598213, -2.77365335598740, 0.20118018545392
C, 5.39385480282667, -3.61020385503000, -0.17572392326784
C, 6.64337165535239, -3.00066199671585, -0.35986440688022
H, 7.49725142007871, -3.62821004847989, -0.62301600993586
H, 3.67238761619920, -0.79635171905342, 0.66481611614529
H, 3.32947889307659, -3.17806388637949, 0.34708970572977
C, 10.86216957477688, 3.22922683177752, -0.69072279366799
C, 11.78687148628663, 2.72162564447921, -1.61402600492894
C, 11.20240819392139, 4.42781629111244, -0.03509761388660
C, 12.39965346918662, 5.07955798109607, -0.28925893450556
C, 12.99643608464647, 3.36319683147314, -1.87906528475446
C, 13.31425669325752, 4.55450941062157, -1.21503944705528
O, 14.45116844122184, 5.24953165766178, -1.39891830052609
C, 15.40380628729009, 4.75738720906969, -2.30862373522087

H, 11.55550757275063, 1.80655764208613, -2.16504913608295
H, 13.67800761515225, 2.93062025134578, -2.61261154854546
H, 10.52204557979544, 4.85135113800216, 0.70787346171148
H, 12.65566549060293, 6.00434299048734, 0.23318588850197
C, 5.19137690568062, -5.06324664525617, -0.36432705806073
C, 4.12681475533533, -5.73678900025004, 0.26736909156601
C, 3.91884435339323, -7.09591889274641, 0.08792148814629
C, 6.03228515794546, -5.82928795226049, -1.18345638244485
C, 5.83852505426136, -7.19782259103785, -1.37137398367705
C, 4.77348447606439, -7.84634824975549, -0.73422032901364
O, 4.49818951076835, -9.15777902681255, -0.85262842855600
C, 5.32911899665860, -9.95100868502075, -1.66355087245978
H, 3.09131264083211, -7.60460722938526, 0.58869988125109
H, 3.44213915441807, -5.18956867017636, 0.91919058783615
H, 6.85777829608540, -5.34934064944980, -1.71471061542623
H, 6.51826925645352, -7.74520003829021, -2.02574089203719
H, 15.77467837615696, 3.76014837708371, -2.01526963315796
H, 16.24419781491186, 5.46374361638332, -2.29770181148518
H, 15.00146560350040, 4.70145922920387, -3.33483856167189
H, 6.37141434950137, -9.95783081014045, -1.30073260096878
H, 5.31888262039674, -9.61514152937572, -2.71483225300425
H, 4.93266353850752, -10.97370850702663, -1.61637203195040
H, -14.00235489183375, 6.38713839500412, -1.72238243141681
H, -14.78103986442017, 5.60859326733485, -0.30131602822567
H, -15.70930953827441, 5.85499625669202, -1.81213975404929
H, -2.57758992462162, -9.87620698903133, -1.98642269842999
H, -3.17985607220474, -11.36314682484456, -1.19177481546998

H, -2.42533329675906, -10.07257523384492, -0.20642758067821
 C, -0.33734301027496, -2.26690440029623, 1.03599563734372
 Br, 0.39702118418767, -1.30619839848135, -0.53329676403426
 C, 0.28255599438442, -3.65346889210884, 0.95986428702859
 O, 1.33659762139693, -3.96064538891307, 1.45891206599139
 O, -0.48092295734749, -4.47044833680854, 0.25062111635380
 C, 0.01226888771570, -5.80059009437003, 0.00090784740327
 C, -0.22735815207141, -6.72412970181076, 1.16778145753511
 H, 1.08096869841232, -5.73570519398481, -0.25160473551278
 H, -0.53605350494742, -6.13000611899522, -0.89162853879523
 H, 0.35972403878795, -6.42205719833430, 2.04682310864357
 H, -1.29257311806299, -6.74826760963282, 1.44269960368602
 H, 0.07414080239413, -7.74525156708155, 0.88833624901409
 C, -0.08446727932386, -1.53387648959096, 2.31382881721539
 C, 1.21207186551772, -1.25380420566566, 2.76651921776931
 C, -1.17989134430708, -1.14009581355961, 3.09044750031825
 C, 1.40413253896955, -0.60754473485870, 3.98352485255007
 H, 2.07304386276785, -1.54533321301882, 2.16416084212132
 C, -0.98491316163486, -0.48716598376909, 4.30800250761554
 H, -2.19387756809114, -1.34941125745966, 2.73971925621943
 C, 0.30698836462110, -0.22286356334925, 4.75796591265897
 H, 2.41893736455037, -0.39525971417893, 4.32775223586745
 H, -1.84854936654791, -0.17648148543642, 4.90073330154707
 H, 0.46251186909968, 0.29075894532263, 5.70985099110851
 H, -1.41116674774391, -2.33329795721778, 0.82855362409690

³PC*/R–X for PC5

charge = 0, multiplicity = 3

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C, 3.20270927506464, -1.58218827966297, -0.50596612505032
C, 2.26408600514016, -0.78918551298321, -1.15074136027707
C, 0.95682284915112, -1.34456481323243, -1.43444116831963
C, 0.65935791434805, -2.62031813054651, -0.97699812558590
C, 1.56629932000086, -3.40378248802860, -0.24985118516669
C, 0.32337580526983, 0.72448932583257, -2.49943936148982
C, 1.60707040167583, 1.26724927344679, -2.22650755227416
C, 1.87251004185948, 2.59132173515759, -2.59952544092749
C, 0.92675468728502, 3.38678392925049, -3.23890779355421
C, -0.34147671129920, 2.82193115908304, -3.56549242566227
C, -0.61507459683784, 1.51512598956983, -3.17473200488338
N, 0.02792042657652, -0.55578153625963, -2.08247492164993
C, -1.30030020657999, -1.05790828407850, -2.25430684983662
C, -2.26644427100937, -0.75281086111654, -1.29549064702609
C, -1.60279587428959, -1.84911856130529, -3.35847585629755
C, -3.55491475454392, -1.24946167214540, -1.44653375021470
C, -2.89392684173941, -2.35128522566028, -3.50463904404649
C, -3.86310698465974, -2.05165077276806, -2.54869003993381
H, 4.20908632053562, -1.18303208415459, -0.38651507370801
H, -0.36204036429002, -2.97769542643100, -1.09908487798804
H, 2.83659429000595, 3.02649679822844, -2.33610136174854
H, -1.58225758200000, 1.07959546025760, -3.42626933792099
H, -2.00325312025601, -0.13364466317267, -0.43570167556729
H, -0.82955246282851, -2.07208005938041, -4.09601102453126
H, -4.31649682810198, -1.01597752244191, -0.69941016031415

H, -3.14121309183463, -2.97544338188637, -4.36467498104894
C, -3.43622889480664, -1.05580291976451, 2.31518608762989
C, -2.56146740512902, 0.01590225728409, 2.47652850919009
C, -1.18038040823557, -0.16467041940623, 2.32098961522196
C, -0.68891418747430, -1.43627112778420, 1.99978532152861
C, -1.56589007694445, -2.50904161368195, 1.84997110289592
C, -2.93919880704539, -2.32216312067404, 2.00308267782665
H, -4.51132251379848, -0.90138435081206, 2.43651432598302
H, -2.95062210166800, 1.00719014189776, 2.72484657392097
H, 0.38132028322624, -1.59209333202624, 1.85667731140209
H, -1.17083464143804, -3.49617199251078, 1.59958168111934
H, -3.62399425313519, -3.16403257776468, 1.87368715559133
C, -0.27626189336347, 1.02374140198353, 2.48554477651618
H, -0.77364978059587, 1.78723690011125, 3.09365253430983
Br, 0.03853063508093, 1.91092564583252, 0.74892082871880
C, 1.02967406978559, 0.69219832002850, 3.18502686357236
O, 1.15861239325919, 0.85287531310437, 4.37199368573565
O, 1.95252142574319, 0.18666340662595, 2.38196396238054
C, 3.17760382115104, -0.27408869376546, 2.97826910214348
C, 3.02028007826192, -1.65024420924449, 3.57211799412856
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H, 3.99006657305498, -1.99206859063928, 3.96403063944961
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C, 3.79762185149960, 1.07864427782767, -1.20712561849285

C, 4.85688217684677, 1.01145958859316, -2.10785875200873
C, 3.94129254519761, 1.69292755825480, 0.03582659807937
C, 6.08264647789995, 1.57248088421935, -1.75976495048189
H, 4.71987003513792, 0.52014479860801, -3.07306671745726
C, 5.16651364064171, 2.25027043795320, 0.38243564723477
H, 3.09052193874956, 1.72397490169523, 0.71839356208466
C, 6.23343285043276, 2.18851025697308, -0.51749206672788
H, 6.92074357429400, 1.52462772703565, -2.45711273529236
H, 5.28964775667614, 2.72988337174899, 1.35572294197780
C, -5.25894594484122, -2.59251186440799, -2.67143552415985
C, 7.53761050457922, 2.83779686304382, -0.15067730262850
F, -5.43788514725244, -3.30010162778188, -3.78845859498165
F, -6.17017649470309, -1.61012469374028, -2.67400405427393
F, -5.56633459363945, -3.39425507887782, -1.64184663134837
F, 7.50216805977775, 4.16308141121772, -0.35443675668804
F, 8.55957888591176, 2.36222672570838, -0.86696526685284
F, 7.83735116231599, 2.65763925575527, 1.14076853573285
C, 4.05585239528743, -3.73117443158800, 0.33142758309625
C, 4.07065502627803, -5.12146968140596, 0.14469380151644
C, 5.19249458079058, -3.14697135127242, 0.97933214192263
C, 5.14357455922311, -5.92829176648694, 0.58818869697961
H, 3.24990366761345, -5.60987880288467, -0.38150965621525
C, 6.24175537618201, -3.90554367285275, 1.42632398337045
H, 5.20791079118226, -2.07004520624875, 1.16260514178873
C, 6.25797697670065, -5.32159255086242, 1.25268714014730
C, 5.15151967005561, -7.33836379138261, 0.40258790411240
H, 7.08166547683958, -3.42886637086299, 1.93952452582999

C, 7.32044724194299, -6.13428330854710, 1.70699370139154
C, 6.20489751660789, -8.10576804121719, 0.85415284445165
H, 4.30186116738416, -7.80567984774698, -0.10343068874927
C, 7.29914245668108, -7.50366301579179, 1.51334680279998
H, 8.16515747377998, -5.66023570214726, 2.21541682446574
H, 6.19357681653508, -9.18872456467816, 0.70376408448361
H, 8.12758586363555, -8.12175141668722, 1.86865735955355
C, 1.05785519176256, -4.57302652294354, 0.44891864800253
C, 1.58912428563418, -5.00195098363612, 1.67377653753477
C, -0.05290339566948, -5.31103830400768, -0.07481758886844
C, 1.06141213249441, -6.10983286275369, 2.37612551041844
H, 2.41162474806284, -4.45495439472706, 2.13389237727456
C, -0.57877556852132, -6.39326940612950, 0.58005399733407
H, -0.47665856009510, -5.02462864388750, -1.04019516507126
C, -0.04574423762786, -6.83381858476518, 1.82784849783162
C, 1.59923523824917, -6.53469219482275, 3.62204184558420
H, -1.41525290129184, -6.94462231257332, 0.14150202628991
C, -0.56445377040803, -7.94387965564396, 2.53127030680495
C, 1.06941670885315, -7.62022675467301, 4.28780055277969
H, 2.44518326768970, -5.98387327247449, 4.04328243520309
C, -0.01977770120632, -8.33397869402740, 3.74118960701537
H, -1.40896683947772, -8.49105771099777, 2.10225434934854
H, 1.49542390016138, -7.93319623430918, 5.24490116445843
H, -0.43058052194161, -9.19357961935357, 4.27683140426568
C, -1.37375290918107, 3.55594757065778, -4.33212475719987
C, -1.05474440982569, 4.25620594513861, -5.48231664458728
C, -2.72793523676485, 3.53802934540026, -3.89448053866753

C, -2.03753255969734, 4.96759525052316, -6.21138424857236
H, -0.02561468921578, 4.27072455255426, -5.84873179666589
C, -3.70472152535916, 4.21794616554660, -4.58168533987809
H, -2.98467303881729, 2.99107533924598, -2.98361870216359
C, -3.39260868384056, 4.95570200577033, -5.75320570007295
C, -1.71443700108991, 5.70189567971605, -7.38430467755916
H, -4.73831388553424, 4.20529222421103, -4.22534036289580
C, -4.37258438920788, 5.67917479754997, -6.48120825672554
C, -2.68718095674559, 6.39407562148112, -8.06821474636996
H, -0.67708234622437, 5.70984744342313, -7.73001637361629
C, -4.02799256917466, 6.38283265805318, -7.61328125858352
H, -5.40677956118386, 5.66783271384670, -6.12612455926884
H, -2.42736476831524, 6.95806706323269, -8.96778086120713
H, -4.79030338344826, 6.93723640591410, -8.16663876566627
C, 1.26686870074506, 4.80347203913328, -3.50349944647331
C, 0.39335929783542, 5.82450673572655, -3.17231936532431
C, 2.51951584663897, 5.13695186062104, -4.09051788310378
C, 0.71053329837075, 7.18039587308430, -3.42637433790389
H, -0.56643456750745, 5.59502313920015, -2.70348809063450
C, 2.85607224127236, 6.44412702871897, -4.34947849275608
H, 3.21164649097065, 4.33433081857462, -4.35736323086068
C, 1.96543111667663, 7.50267849719661, -4.03288882999331
C, -0.18702063895640, 8.23326185149332, -3.10180144762114
H, 3.81680083659644, 6.68334913346052, -4.81345964010045
C, 2.27476063929246, 8.86255097313390, -4.29576854408776
C, 0.14181587568535, 9.54229876282428, -3.36915829184178
H, -1.14557557868476, 7.98251690322830, -2.63913589324538

C, 1.38328666121412, 9.86019047932026, -3.97138943552318
H, 3.23466424156579, 9.10348224664597, -4.76093513151204
H, -0.55677946916616, 10.34439910210373, -3.11748304138321
H, 1.63120248791016, 10.90450602743468, -4.17796703814288

PC⁺/X⁻ for PC1

charge = 0, multiplicity = 2

C, 2.57576674848402, -3.03163769511541, 0.21554933964432
C, 3.02396124652432, -1.82896575829558, -0.30852121328665
C, 2.15638138131815, -0.99456715759237, -1.02390778082901
C, 0.80652091650424, -1.36015557362447, -1.22350812774973
C, 0.37505690147209, -2.58762979765340, -0.68370470080317
C, 1.24345482787717, -3.40669905070384, 0.02050247741512
C, 0.16438004571227, 0.74209669362568, -2.30832355125130
C, 1.45519115959998, 1.33282844691496, -2.19883291301100
C, 1.67448001463362, 2.65227253110394, -2.62419950802786
C, 0.64591758368754, 3.39536279297335, -3.17026501974506
C, -0.62820559660334, 2.82123998871072, -3.29688303476697
C, -0.86737760580322, 1.53070353128161, -2.87227460172415
S, 2.85662150067512, 0.44951142438887, -1.69887585944903
N, -0.08674578432369, -0.55930739011267, -1.93316685085388
C, -1.43932784920777, -1.03243325986908, -2.05023512875326
C, -2.35069969417657, -0.72073630377643, -1.04115467276026
C, -1.81008403149053, -1.79014425381609, -3.15745844162895
C, -3.66001154945571, -1.18408499703952, -1.14837966481772
C, -3.12340605058187, -2.24932136747642, -3.25422091781948
C, -4.04561646034796, -1.94817549426405, -2.25177196203718

H, 3.26051456767201, -3.67358444017076, 0.77347393152502
 H, 4.06267857044199, -1.51872991351615, -0.16619036546784
 H, -0.65970542606657, -2.89863361275588, -0.82074905006000
 H, 0.87227299297986, -4.35068069414651, 0.42556230649307
 H, 2.67543468106260, 3.07993186969033, -2.52504921150819
 H, 0.82787763090234, 4.41987013964818, -3.50140121698673
 H, -1.44768199017125, 3.39852723671651, -3.73073346307621
 H, -1.86477882492304, 1.10670784376604, -2.97635458375889
 H, -2.01505427818302, -0.10584210304090, -0.19960828979921
 H, -1.07245699702155, -2.01505101409283, -3.93093975799893
 H, -4.38479328480623, -0.94586342481657, -0.36594692128188
 H, -3.42625734714574, -2.84496759876152, -4.11875835606245
 H, -5.07374873236119, -2.31011886770718, -2.33163460897883
 Br, 0.01173444720684, 1.79332154990153, 0.60530125642990

PC⁺/X⁻ for PC2

charge = 0, multiplicity = 2

C, -3.07283491462460, 1.03441565032621, 0.85182576830656
 C, -1.82624882518011, 0.43276386582861, 0.59165576460018
 C, -0.92040121431027, 1.09112089606579, -0.28930192423457
 C, -1.29863385142719, 2.33368210510915, -0.88444921323644
 C, -2.56017039125556, 2.89350429638833, -0.59257037957422
 C, -3.43381175421591, 2.24553194176639, 0.26868555724573
 H, -3.78350509851563, 0.55395667322253, 1.52423097624737
 C, 0.35728791562110, 0.53450419623327, -0.59096091506786
 C, -0.40417586562168, 2.99037458176836, -1.76232299898194
 H, -2.83627247554571, 3.84401202984621, -1.05561060442068

H, -4.40905829190759, 2.68198475401316, 0.49355296147057
 C, 0.83443474435719, 2.43759601723899, -2.04448217368710
 C, 1.21849061332081, 1.22883796056595, -1.46673360186830
 H, -0.70925845349014, 3.94012275429229, -2.20876710547192
 H, 1.52479430706194, 2.94598022594263, -2.72145708410884
 H, 2.21360336238498, 0.83236358105191, -1.72219470180882
 C, -1.44049450715261, -0.82953013533059, 1.19130469068219
 C, -0.16407520330935, -1.38510889549987, 0.88782355383558
 C, -2.29025510860330, -1.53026519309059, 2.06879942840095
 C, 0.74133389362182, -0.72506907653073, 0.00569402237465
 C, 0.21744049051662, -2.62898143314519, 1.47814053391299
 C, -1.91147087073903, -2.74171986211414, 2.64051419409998
 H, -3.27226941563100, -1.12815567816295, 2.31673852932153
 C, 1.99231070609799, -1.31931328505673, -0.26347725110698
 C, 1.48307803530796, -3.18507008198469, 1.18050779821422
 C, -0.67091048285017, -3.29099208120787, 2.35251714605938
 H, -2.59730319156061, -3.25580782030297, 3.31688491171463
 C, 2.35180273902746, -2.53241870160138, 0.31974188303079
 H, 2.71632335795811, -0.84320567043914, -0.94237995074584
 H, 1.76059666078720, -4.13660125848897, 1.64095642309674
 H, -0.36438029995655, -4.24102824659639, 2.79688344429289
 H, 3.32807486779768, -2.96559768379436, 0.09052525141969
 Br, 4.42148991203614, 0.09809136368677, -2.55061228401312

PC⁺/X⁻ for PC3

charge = 0, multiplicity = 2

C, -0.09071795742531, -3.82303446765199, 0.87526745460057

C, -1.75918205461065, -3.93226921840797, -0.93538582791300
C, 0.16668415431386, -3.05398581639549, 2.01448165986099
C, 0.29774519949176, -5.17004227217474, 0.83914371459877
C, -2.01074787201882, -3.63607689444589, -2.28242947909855
C, -2.53348663431061, -4.90895595841610, -0.29410175821754
C, 0.83541606119045, -3.62260658381156, 3.09653615637979
H, -0.14806468018363, -2.00357381504203, 2.07098983614985
C, 0.93993919144491, -5.73262574820044, 1.93739684489595
C, -3.01209263613685, -4.31298846424145, -2.97318715917316
H, -1.43641780321556, -2.86199468653172, -2.79212389701121
C, -3.51989546853145, -5.59072226181207, -0.99865480122386
C, 1.22199689944700, -4.96147906832597, 3.06747590886023
H, 1.04102866144227, -3.00188856904134, 3.97254138652643
H, 1.23905833725260, -6.78316902850447, 1.90051155140469
C, -3.76650481389441, -5.30059687397294, -2.34171744989434
H, -3.19485676922705, -4.06604892206620, -4.02197611025174
H, -4.11552968408864, -6.34793498482593, -0.48253606982973
H, 1.73680535371190, -5.40696748506685, 3.92222197622098
H, -4.54672976288118, -5.83515544910357, -2.88845293766071
C, -0.50789930785148, -1.88630063722444, -0.52987629699384
C, 0.80582473560746, -1.42211495345752, -0.81687209684181
C, -1.58092558821995, -0.97277888045349, -0.55289772516391
C, 1.01163213787046, -0.06372477104679, -1.17069242952110
C, -1.40275270867654, 0.37341734728088, -0.95346781475357
C, -0.08913710528702, 0.80750930290188, -1.24950656163125
N, -0.75102721942460, -3.23011296025167, -0.23004008847639
C, 0.14149124691785, 2.15334513795694, -1.65960524567741

N, 0.34948649618215, 3.24550006138886, -1.98904379964210
C, -2.87512269069626, -1.44317102256717, -0.18316035003607
N, -3.91725158970393, -1.84317460388121, 0.13109095710269
N, 2.29060702547193, 0.38570668437300 -1.52874967795448
C, 2.88138260304953, -0.18509137905291, -2.68605285943798
C, 2.85394437763941, 1.51286092923234, -0.89170470320875
C, 2.08696947868324, -0.44032573288946, -3.81024714026466
C, 4.24987271328058, -0.48291129765618, -2.72214335905137
C, 2.47356892127162, 1.83168486533858, 0.42007493897158
C, 3.77218751590565, 2.33688929767300, -1.55978220928734
C, 2.64910094204741, -1.02071106210425, -4.94541289132267
H, 1.02692097873135, -0.17695593868371, -3.79569203995242
C, 4.80424483315594, -1.05023369238554, -3.86526481440698
C, 3.02190456905437, 2.94387939423653, 1.05160937376253
H, 1.72291865651381, 1.24221747710809, 0.96048024504254
C, 4.32396843312871, 3.43579978104066, -0.90836330112431
C, 4.00737361669033, -1.33135862522228, -4.97701262326105
H, 2.01705632211111, -1.22214344567109, -5.81372163945133
H, 5.87183060122637, -1.28329172804913, -3.88227925192292
C, 3.95900651424761, 3.74710761351625, 0.40274098661211
H, 2.70553648128376, 3.17266245734463, 2.07279259301979
H, 5.03984487360106, 4.06542510536616, -1.44314367927582
H, 4.44799932064504, -1.78384185942720, -5.86852617852118
H, 4.39374832086216, 4.61332134629708, 0.90714356882962
N, 1.90254839653599, -2.29986862456906, -0.76989712295216
C, 2.99329692832015, -1.98718340162015, 0.05594866242540
C, 1.89545274003439, -3.46628879386542, -1.55017886899080

C, 2.77386141120929, -1.25866774259808, 1.23808013635917
C, 4.29693811283763, -2.40147209623131, -0.28338495430008
C, 1.23391314679751, -3.46567025010712, -2.78975400869297
C, 2.54862810088221, -4.63190915514153, -1.10660915097718
C, 3.84415312772204, -0.96298924465250, 2.07074309311782
H, 1.77000867465415, -0.92728845920537, 1.52987875308791
C, 5.35222496518481, -2.10441721766366, 0.56546659649969
C, 1.23914310425774, -4.60710235075532, -3.57796122594745
H, 0.74512368065668, -2.55755231854886, -3.13966803618446
C, 2.55787032283727, -5.76174850244367, -1.91196827500342
C, 5.13361883884966, -1.38720601116141, 1.74664616808039
H, 3.65506931435946, -0.39946443750399, 2.98739075500387
H, 6.36207217267601, -2.41953628689756, 0.29350048710621
C, 1.90558977466456, -5.75703255303883, -3.14736087039880
H, 0.72962892461626, -4.59357372817749, -4.54391215799977
H, 3.06117301136135, -6.66488337149962, -1.55984661960468
H, 5.97157839012699, -1.15609627249720, 2.40850330631350
H, 1.91330006797768, -6.65193027119434, -3.77382398591586
H, 4.87666998059597, -0.26349911332658, -1.85771652632427
H, 4.04771300883839, 2.12904999113541, -2.59438909031788
H, 3.02065568670917, -4.65562816157026, -0.12501331712532
H, 4.48153681339936, -2.92604786770237, -1.22048030417205
H, -2.37514993795286, -5.12347546182934, 0.76363387630915
H, 0.09739767514558, -5.77345044834751, -0.04685956048054
N, -2.47772684423180, 1.23566262781646, -1.10592346265891
C, -3.48168738047541, 1.32563126612283, -0.11086548134043
C, -2.60180162501177, 1.97810915216600, -2.30712302686501

C, -3.11261631155990, 1.29838756443235, 1.23808559157085
 C, -4.83116937564168, 1.42412368306169, -0.47434830391132
 C, -2.29991794949571, 1.36695674805409, -3.52991177361842
 C, -3.01497779808741, 3.31510610725195, -2.27331613088665
 C, -4.10072397124190, 1.34267753348716, 2.21812137934202
 H, -2.05720020093219, 1.21653831917338, 1.53292242583942
 C, -5.80471270381054, 1.48627502107424, 0.51616717543305
 H, -5.11449738286034, 1.43028860318301, -1.52862427790239
 C, -2.38150132242733, 2.10281627493737, -4.70922307824542
 H, -2.00311687660958, 0.31556673274821, -3.55266284818484
 C, -3.10980425729572, 4.03488964583228, -3.45889094465243
 H, -3.23936135524931, 3.78974935583858, -1.31609399204564
 C, -5.44664143370000, 1.43965890889368, 1.86639385321556
 H, -3.80371384627913, 1.30765634499839, 3.26961449792643
 H, -6.85722258376399, 1.55598489909607, 0.23019103859349
 C, -2.78653241740805, 3.43694182486278, -4.67960522036013
 H, -2.13955502752045, 1.62187933308288, -5.66015630689035
 H, -3.42438956842168, 5.08094763519533, -3.42773026683970
 H, -6.21782873233968, 1.47979993252901, 2.63960289860411
 H, -2.85434279940110, 4.01121010100327, -5.60656730302622
 Br, 0.04165010337719, 0.48737189318035, 2.78101691260326

PC⁺⁺/X⁻ for PC4

charge = 0, multiplicity = 2

C, 4.81769868489986, 0.75813911107528, 1.63910095253048
 C, 4.92949305470361, 0.46791339654468, 0.27895879832219
 C, 3.80754544957649, 0.43588255754511, -0.54297756833453

C, 3.56332690141591, 1.01429489432019, 2.17649086054832
C, 2.41543928949451, 0.97488894084989, 1.36992461251298
C, 2.55336174669696, 0.68872247080357, 0.00461279618579
C, 1.08931162535751, 1.23983798190210, 1.97766656374054
H, 3.45576252559317, 1.23958226846724, 3.23852598550321
H, 5.72446239515183, 0.78127067052436, 2.25138337546305
N, 6.22597272936525, 0.19353339625803, -0.26646455615709
H, 1.68122444018061, 0.67591097355058, -0.65137382985334
H, 3.92067571973899, 0.21721303352726, -1.60670502073619
C, -0.10392354119831, 0.87148535655024, 1.34955685435560
N, 1.07476689403959, 1.83538632696059, 3.17289784107313
C, -0.10547132577920, 2.06978804718368, 3.74521349275142
N, -1.28577643921685, 1.76147282652616, 3.20881770886783
C, -1.29881767686977, 1.16656646141955, 2.01313897258557
H, -0.10323150921630, 0.34383810017098, 0.39728849882846
C, -2.62188282093755, 0.82186518211308, 1.44185215685567
C, -0.10587040133013, 2.72851791122020, 5.07558750077615
C, -2.78814086621117, 0.57463583937937, 0.07149921430346
C, -4.03994995598970, 0.25248632015099, -0.44165687707359
C, -3.73987341026705, 0.74370173914091, 2.28491980325372
C, -4.99032031412410, 0.41577386573631, 1.77534073912889
C, -5.14243557561748, 0.16940566608326, 0.40971350762305
H, -1.94067975348661, 0.65123101805247, -0.61245745297347
H, -4.17122287869174, 0.06767851308966, -1.51002124784012
H, -3.61359862096520, 0.93352418956433, 3.35187914607951
H, -5.85892306176236, 0.34547755215677, 2.43380367032982
C, 1.10189822330511, 3.08089924575398, 5.69443144221369

C, 1.10023590455037, 3.69823160288010, 6.94225267831956
C, -0.10668661366933, 3.97223059443433, 7.58779638294598
C, -1.31321788642750, 3.62495745940358, 6.97773866901678
C, -1.31410657708322, 3.00770911103094, 5.72985922910275
H, -2.25369712143603, 2.73565697578819, 5.24598414747034
H, -2.26130621827272, 3.83819579045932, 7.47803876071185
H, 2.04178087881352, 2.86504075597830, 5.18357445446221
H, 2.04793889663894, 3.96855010670699, 7.41491756362112
H, -0.10699262289134, 4.45683257122209, 8.56762692666963
N, -6.42400974784702, -0.16572831745482, -0.11466417220778
C, -7.27162459093576, 0.85420439381521, -0.53879383045239
C, -6.80275372239568, -1.50419628699231, -0.17538378645078
C, -8.06542469615515, -1.87710204476771, -0.67585052301396
C, -8.54847762636038, 0.56465984869129, -1.05807961632066
C, -9.08206856404745, -0.85941053480643, -1.18573736225622
C, -6.85716762526760, 2.19664523143544, -0.45464533999577
C, -7.68188951633836, 3.22985523644511, -0.87107544327169
C, -8.95915385568497, 2.97201408504427, -1.39026451140456
C, -9.35340091904038, 1.62972536679511, -1.46697488682258
C, -5.92139838382402, -2.50748374236014, 0.26921278158582
C, -6.27585438753014, -3.84653025206125, 0.22262775701819
C, -7.52575218543953, -4.24793271215551, -0.27146908294030
C, -8.38876444575801, -3.23495951082845, -0.71015692627638
C, -10.37660207384745, -0.98898625752165, -0.36335676665556
H, -11.14217304119923, -0.28264032632660, -0.71798552725957
H, -10.79769170412833, -2.00200493527571, -0.44859740991575
H, -10.18773746199663, -0.78448324750247, 0.70166766819282

C, -9.38415837060666, -1.14829727438951, -2.66706894542229
H, -8.47241868727259, -1.06227143521418, -3.27790297588980
H, -9.78957247704956, -2.16307451178024, -2.79683615875049
H, -10.12895375817762, -0.44077118613301, -3.06176148961207
H, -5.86659401287810, 2.43295734558472, -0.06514843329998
H, -7.31077076604022, 4.25540040001540, -0.80710702222638
H, -10.35066292112006, 1.40132190219175, -1.84885344266908
H, -4.94555284618478, -2.23117515617289, 0.66941800503660
H, -5.56841627082865, -4.58900332003082, 0.59921615123358
H, -9.36016882263099, -3.51983307822639, -1.11962639097338
C, -7.91812248848911, -5.67241552892988, -0.32661282405858
C, -6.96503201316678, -6.68682784378741, -0.49181086617090
C, -7.31995589473110, -8.03427972030353, -0.54390924605848
C, -8.66541665320652, -8.40591725321759, -0.43141943426724
C, -9.26428376924510, -6.06878188603002, -0.21365867270051
C, -9.63411146119399, -7.40422791895970, -0.26511240469243
O, -9.11047182636942, -9.67454713564688, -0.47115865017041
C, -8.17502369746083, -10.71289447888162, -0.62867954598687
H, -5.91007873131122, -6.42499611833422, -0.60475414151279
H, -6.54046646304673, -8.78460928711330, -0.68178556772022
H, -10.04113042307847, -5.31556996618319, -0.06087192332090
H, -10.68144621598947, -7.69943334818408, -0.16721843723100
C, -9.85081287447275, 4.06408958981541, -1.83559260235661
C, -9.80176961675665, 5.33345467383276, -1.24309569735988
C, -10.63543019388746, 6.37375156457148, -1.65210186951492
C, -11.55882786670698, 6.16277584127720, -2.68358619378670
C, -11.62254591423543, 4.89830511857689, -3.28897753811975

C, -10.78501035071021, 3.87479711110416, -2.87173462140966
H, -12.33729323361347, 4.74186035452720, -4.10034199744747
H, -10.84482402609413, 2.90891539095359, -3.37957069403614
H, -9.10689607239238, 5.51991288297225, -0.42044544432021
H, -10.56270917025626, 7.34087386784753, -1.15308910114867
O, -12.40729002143639, 7.09709012609733, -3.14849581162191
C, -12.37094924178271, 8.38343233274916, -2.58111368447427
C, 6.71736366551687, -1.10088586215336, -0.16344002383418
C, 8.02562190768686, -1.40486050490090, -0.60088716775108
C, 8.85304343347944, -0.37591852899145, -1.34988527677508
C, 7.04212658017224, 1.25084818192390, -0.57922382456518
C, 8.37012376612308, 1.02693139939106, -1.03661638232438
C, 6.56453968275525, 2.57770017455987, -0.45684647490464
C, 7.37250183121443, 3.64599403958069, -0.76549920847860
C, 9.15077180056562, 2.13596885669606, -1.35265456903253
C, 8.69663430497524, 3.45322621516870, -1.22315403160586
H, 5.54338313739448, 2.75714446140189, -0.12257041940125
H, 6.96370101335759, 4.65417242945577, -0.67578363408284
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PC⁺/X⁻ for PC5

charge = 0, multiplicity = 2

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