Electronic Supplementary Information for

Theoretical design of phosphorus-doped perylene derivatives as efficient singlet fission chromophores

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angle (Fig. S3).

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The solvation effects were evaluated by polarizable continuum model (PCM)[1] with toluene and chloroform used as solvents. The calculated $E(S_1)_V$ with functional B3LYP are closer to the experimental values for perylene. Moreover, the basis set was extended to larger basis sets, including 6-311G** and cc-pVTZ. The calculated results show that solvation effects affect the SF relevant excited state energies (Table S2), while the excitation energies are insensitive to the extension of basis set (Table S1). The dispersion function also has a negligible impact on the excitation energy, thus allowing the calculation of the exciton binding energy (E_{bin}) using the vertical excitation energies computed at the B3LYP/6-311G* level (Table S3) .

Table S1. Vertical excitation energies [eV] of perylene with different basis sets at B3LYP.

		6-311G*	6-311G**	cc-PVTZ	Exp
Perylene	$E(S_1)$v	2.856	2.848	2.801	2.820[2]
	$E(T_1)$v	1.549	1.547	1.534	1.530[3]

Table S2. Solvation effects on vertical excitation energies [eV] of S_1 and T_1 states for Perylene.

Molecule		Vacuum	Toluene	Dichloromethane	Exp
Perylene	$E(S_1)$v	2.856	2.753	2.667	2.820[2]
	$E(T_1)$v	1.549	1.554	1.560	1.530[3]

Table S3. Comparison of Vertical Excitation Energies $E(S_1)_V$ and $E(T_1)_V$ at B3LYP/6-311G* and B3LYP/6-311+G* levels

	$E(S_1)_V$		$E(T_1)_V$	
	6-311G*	**6-311+G***	**6-311G***	**6-311+G***
PP2-a	2.514	2.474	1.284	1.262
PP2-b	2.460	2.428	1.214	1.192
PP2-Cs	2.503	2.466	1.251	1.230
PP3	2.393	2.361	1.184	1.160
PP4	2.322	2.290	1.148	1.122

Table S4. Comparison of vertical excitation energies $E(S_1)_V$ and $E(T_1)_V$ at TD-DFT and CASPT2//CASSCF(12,11) level.

Molecule	CASPT2(12, 11)			TD-B3LYP			$\Delta E(S_1)$v	$\Delta E(T_1)$v	y_0[a]
	$E(S_1)$v	$E(T_1)$v	ΔE_{SF}v	$E(S_1)$v	$E(T_1)$v	ΔE_{SF}v			
PP1	2.969	1.665	-0.361	2.63	1.365	-0.100	-0.339	-0.300	0.250
PP2-a	2.783	1.477	-0.171	2.514	1.284	-0.054	-0.269	-0.193	0.274
PP3	2.585	1.331	-0.077	2.393	1.184	0.025	-0.192	-0.147	0.301
PP4	2.405	1.249	-0.093	2.322	1.148	0.026	-0.083	-0.101	0.318

a: y_0 is calculated at UNO/6-31G* level.

Table S5. Comparison of vertical excitation energies $E(S_1)_V$ and $E(T_1)_V$ at TD-DFT and TDA-DFT methods.

Molecule	TD-DFT		TDA-DFT		Exp	
	$E(S_1)$v	$E(T_1)$v	$E(S_1)$v	$E(T_1)$v	$E(S_1)$v	$E(T_1)$v
Perylene	2.856	1.549	3.021	1.734	2.820	1.530
BP1	2.547	1.304	2.776	1.539		
BP2-a	2.376	1.187	2.599	1.423		
BP2-b	2.409	1.223	2.624	1.450		
BP2-Cs	2.389	1.178	2.620	1.411		
BP3	2.300	1.154	2.511	1.382		
BP4	2.243	1.147	2.439	1.369		
OP1	2.775	1.532	2.980	1.773		
OP2-a	2.723	1.524	2.918	1.766		
OP2-b	2.735	1.544	2.922	1.785		
OP2-Cs	2.770	1.548	2.971	1.791		
OP3	2.731	1.555	2.912	1.801		
OP4	2.738	1.577	2.909	1.830		
PP1	2.630	1.356	2.663	1.592		
PP2-a	2.514	1.283	2.735	1.517		
PP2-b	2.460	1.213	2.686	1.447		
PP2-Cs	2.503	1.250	2.735	1.485		
PP3	2.393	1.183	2.612	1.415		
PP4	2.322	1.147	2.532	1.377		

Table S6. Comparison of Vertical Excitation Energies $E(S_1)_V$ and $E(T_1)_V$ using different exchange-correlation functionals.

Molecule	PBE0		CAM-B3LYP		ω-B97XD		M06-2X	
	$E(S_1)$v	$E(T_1)$v	$E(S_1)$v	$E(T_1)$v	$E(S_1)$v	$E(T_1)$v	$E(S_1)$v	$E(T_1)$v
Perylene	2.932	1.426	3.167	1.351	3.200	1.492	3.185	1.892
BP1	2.617	1.171	2.811	1.021	2.851	1.171	2.832	1.600
BP2-a	2.443	1.046	2.631	0.843	2.674	1.004	2.647	1.466
BP2-b	2.476	1.085	2.646	0.886	2.685	1.033	2.662	1.481
BP2-Cs	2.456	1.038	2.632	0.834	2.673	0.993	2.649	1.449
BP3	2.366	1.012	2.539	0.776	2.581	0.932	2.549	1.406
BP4	2.309	1.005	2.483	0.750	2.526	0.903	2.487	1.389
OP1	2.854	1.406	3.108	1.314	3.146	1.461	3.121	1.876
OP2-a	2.804	1.393	3.073	1.283	3.115	1.435	3.082	1.873
OP2-b	2.816	1.413	3.089	1.310	3.131	1.462	3.095	1.889
OP2-Cs	2.851	1.416	3.114	1.312	3.155	1.463	3.122	1.892
OP3	2.815	1.418	3.098	1.298	3.143	1.455	3.102	1.906
OP4	2.825	1.433	3.122	1.300	3.169	1.461	3.122	1.936
PP1	2.702	1.221	2.918	1.075	2.957	1.219	2.934	1.653
PP2-a	2.585	1.143	2.805	0.965	2.847	1.106	2.811	1.565
PP2-b	2.530	1.068	2.735	0.863	2.777	1.014	2.750	1.484
PP2-Cs	2.572	1.108	2.780	0.918	2.824	1.067	2.788	1.526
PP3	2.462	1.036	2.673	0.812	2.720	0.961	2.676	1.445
PP4	2.390	0.997	2.607	0.751	2.657	0.900	2.602	1.401

Table S7. Torsion angles of P-doped perylenes.

Molecule	φ	φ’
Perylene	0	0
BP1	12.401	9.836
BP2-a	19.171	19.171
BP2-b	27.046	15.344
BP2-Cs	18.023	18.023
BP3	30.445	22.268
BP4	32.638	32.638
OP1	11.964	9.571
OP2-a	16.973	16.973
OP2-b	-19.999	-14.396
OP2-Cs	-17.055	-17.055
OP3	23.507	20.628
OP4	26.457	26.457
PP1	11.691	-9.541
PP2-a	-16.830	-16.830
PP2-b	-19.175	-14.521
PP2-Cs	-16.696	-16.696
PP3	-22.747	-20.536
PP4	-25.833	-25.833

Table S8 The contribution of the $3p_z$ orbital of the P atom to the HOMO and LUMO in P-doped perylenes.

Molecule	HOMO%	LUMO%
BP1	14.115	19.803
BP2-a	22.400	22.600
BP2-b	26.040	32.140
BP2-Cs	25.890	31.824
BP3	32.930	37.443
BP4	39.180	43.086
OP1	2.846	5.447
OP2-a	4.033	10.700
OP2-b	6.437	8.161
OP2-Cs	6.415	7.159
OP3	9.390	11.251
OP4	10.176	13.206
PP1	15.406	21.354
PP2-a	24.879	31.268
PP2-b	27.915	37.221
PP2-Cs	28.065	31.936
PP3	35.688	42.222
PP4	42.198	48.358

Table S9 HOMO, LUMO energy levels and HLG values [eV], diradical character y_0 and tetraradical character y_1.

Molecule	HOMO	LUMO	HLG	y_0	y_1
Perylene	-5.192	-2.152	3.039	0.212	0.022
BP1	-5.281	-2.534	2.747	0.256	0.034
BP2-a	-5.400	-2.804	2.595	0.284	0.052
BP2-b	-5.409	-2.770	2.640	0.277	0.035
BP2-Cs	-5.396	-2.814	2.582	0.288	0.042
BP3	-5.530	-2.996	2.533	0.298	0.053
BP4	-5.658	-3.159	2.499	0.307	0.057
OP1	-5.432	-2.433	2.999	0.218	0.038
OP2-a	-5.669	-2.697	2.972	0.222	0.048
OP2-b	-5.667	-2.670	2.997	0.219	0.043
OP2-Cs	-5.675	-2.665	3.010	0.219	0.047
OP3	-5.900	-2.895	3.005	0.220	0.050
OP4	-6.123	-3.090	3.034	0.219	0.052
PP1	-5.308	-2.520	2.789	0.250	0.029
PP2-a	-5.415	-2.737	2.678	0.274	0.032
PP2-b	-5.431	-2.832	2.600	0.284	0.034
PP2-Cs	-5.429	-2.790	2.639	0.279	0.043
PP3	-5.533	-2.997	2.536	0.301	0.044
PP4	-5.634	-3.165	2.469	0.318	0.047

Table S10. Comparison of HOMO, LUMO energies and corresponding HLG using different exchange-correlation functionals.

compound	PBE0			CAM-B3LYP			M06-2X			ωB97XD			Exp[4]		
	HOMO	LUMO	HLG	HOMO	LUMO	HLG	HOMO	LUMO	HLG	HOMO	LUMO	HLG	HOMO	LUMO	HLG
perylene	-5.394	-2.068	3.326	-6.326	-1.121	5.206	-6.289	-1.468	4.822	-6.877	-0.565	6.312	-5.370	-2.450	2.920
BP1	-5.484	-2.459	3.024	-6.384	-1.539	4.846	-6.331	-1.869	4.461	-6.942	-0.986	5.956			
BP2-a	-5.604	-2.738	2.866	-6.482	-1.826	4.657	-6.416	-2.146	4.270	-7.046	-1.279	4.163			
BP2-b	-5.614	-2.702	2.912	-6.492	-1.791	4.701	-6.421	-2.113	4.307	-7.058	-1.245	5.813			
BP2-Cs	-5.601	-2.747	2.854	-6.473	-1.841	4.633	-6.403	-2.157	4.246	-7.038	-1.296	5.742			
BP3	-5.737	-2.936	2.801	-6.594	-2.032	4.562	-6.511	-2.343	4.167	-7.165	-1.494	5.670			
BP4	-5.868	-3.104	2.764	-6.711	-2.203	4.507	-6.615	-2.508	4.107	-7.287	-1.674	5.613			
OP1	-5.642	-2.358	3.284	-6.567	-1.409	5.158	-6.518	-1.746	4.772	-7.122	-0.857	6.265			
OP2-a	-5.888	-2.631	3.256	-6.810	-1.681	5.129	-6.751	-2.009	4.742	-7.371	-1.136	6.235			
OP2-b	-5.885	-2.603	3.282	-6.803	-1.648	5.156	-6.741	-1.978	4.763	-7.365	-1.101	6.264			
OP2-Cs	-5.893	-2.598	3.295	-6.811	-1.643	5.168	-6.749	-1.973	4.776	-7.372	-1.096	6.276			
OP3	-6.126	-2.836	3.290	-7.043	-1.878	5.166	-6.970	-2.200	4.770	-7.611	-1.337	6.274			
OP4	-6.358	-3.038	3.320	-7.276	-2.074	5.201	-7.191	-2.390	4.801	-7.849	-1.538	6.311			
PP1	-5.511	-2.447	3.064	-6.401	-1.524	4.877	-6.346	-1.852	4.494	-6.958	-0.978	5.980			
PP2-a	-5.617	-2.672	2.945	-6.476	-1.755	4.721	-6.409	-2.074	4.335	-7.039	-1.219	5.819			
PP2-b	-5.634	-2.769	2.865	-6.487	-1.860	4.627	-6.415	-2.171	4.244	-7.051	-1.325	5.726			
PP2-Cs	-5.631	-2.726	2.905	-6.486	-1.814	4.672	-6.415	-2.128	4.287	-7.050	-1.278	5.771			
PP3	-5.736	-2.940	2.796	-6.562	-2.031	4.531	-6.480	-2.336	4.144	-7.131	-1.506	5.625			
PP4	-5.838	-3.114	2.724	-6.638	-2.205	4.433	-6.545	-2.502	4.042	-7.212	-1.689	5.523			

Table S11. The HOMA values of each ring of perylene derivatives.

Compound	Ring 1	Ring 2	Ring 3	Ring 4	Ring 5	$HOMA_{avg}$
Perylene	0.773	0.773	0.014	0.773	0.773	0.773
BP1	0.258	0.719	0.008	0.792	0.798	0.642
BP2-a	0.214	0.214	0.021	0.815	0.815	0.515
BP2-b	0.243	0.770	0.088	0.243	0.77	0.507
BP2-Cs	0.295	0.775	0.002	0.775	0.295	0.535
BP3	0.312	0.795	-0.013	0.284	0.277	0.417
BP4	0.265	0.265	0.133	0.265	0.265	0.265
OP1	0.431	0.725	-0.055	0.791	0.793	0.685
OP2-a	0.381	0.381	-0.117	0.810	0.810	0.596
OP2-b	0.451	0.750	-0.112	0.451	0.750	0.601
OP2-Cs	0.456	0.748	-0.105	0.748	0.456	0.602
OP3	0.471	0.770	-0.175	0.404	0.408	0.513
OP4	0.428	0.428	-0.247	0.428	0.428	0.428
PP1	0.259	0.758	-0.001	0.787	0.794	0.650
PP2-a	0.247	0.247	-0.019	0.806	0.806	0.527
PP2-b	0.287	0.783	0.005	0.287	0.783	0.535
PP2-Cs	0.295	0.775	0.002	0.775	0.296	0.535
PP3	0.312	0.795	-0.013	0.284	0.277	0.417
PP4	0.303	0.303	-0.028	0.303	0.303	0.303

Table S12. Calculated SOC (cm^{-1}) for perylene and perylene derivatives at S_1 geometry.

	$SOC(S_1\text{-}T_1)/cm^{-1}$	$\Delta E_{S1\text{-}T1}/eV$	$SOC(S_1\text{-}T_2)/cm^{-1}$	$\Delta E_{S1\text{-}T2}/eV$
Perylene	0	1.181	0	-0.152
BP1	0.090	1.126	0.120	-0.141
OP1	0.152	1.120	0.172	0.100
PP1	0.045	1.170	0.212	-0.015
BP2-a	0	1.066	0.200	0.060
BP2-b	0	1.034	0	-0.347
BP2-Cs	0.12	1.097	0	-0.061
BP3	0.04	1.002	0.100	-0.094
BP4	0	0.953	1.287	-0.049
OP2-a	0.212	1.073	0.509	0.028
OP2-b	0.085	1.054	0.368	0.195
OP2-Cs	0.030	1.087	0.318	0.275
OP3	0.192	1.029	0.772	0.267
OP4	0	0.994	0.948	0.335
PP2-a	0.424	1.113	0.779	0.141
PP2-b	0.170	1.156	1.118	-0.084
PP2-Cs	0.010	1.151	0.930	0.214
PP3	0.456	1.106	0.908	0.153
PP4	0	1.064	0.622	0.194

Table S13. The calculated vertical ionization potential (VIP), vertical electron affinity (VEA), $E_{gap,F}$ and corresponding energy exciton binding energies of perylene.

Molecule	E_{VIP}	E_{VEA}	$E_{gap,F}$	Ebin(S_1)	Ebin(T_1)
BP1	7.590	0.899	5.791	2.935	4.241
BP2-a	8.356	1.506	5.343	2.934	4.120
BP2-b	8.392	1.559	5.274	2.886	4.096
BP2-Cs	8.689	1.747	5.196	2.896	4.042
BP3	8.965	1.919	5.128	2.885	3.981
BP4	8.077	1.190	5.697	2.922	4.164
OP1	8.019	1.271	5.477	2.930	4.172
OP2-a	8.547	1.463	5.621	2.898	4.097
OP2-b	8.522	1.440	5.641	2.907	4.097
OP2-Cs	8.522	1.435	5.653	2.883	4.105
OP3	8.952	1.676	5.600	2.870	4.045
OP4	9.348	1.884	5.580	2.842	4.003
PP1	8.388	1.549	5.289	2.913	4.102
PP2-a	8.032	1.266	5.499	2.869	4.143
PP2-b	8.320	1.484	5.351	2.837	4.067
PP2-Cs	8.441	1.591	5.260	2.799	4.046
PP3	8.401	1.554	5.294	2.791	4.043
PP4	8.682	1.764	5.154	2.761	3.971

Table S14 Vertical excitation energies ($E(S_1)$v and $E(T_1)$v), adiabatic excitation energies ($E(S_1)$, $E(T_1)$ and $E(T_2)$) and ΔE_{SF} and ΔE_{TTA} [eV].

Molecule	$E(S_1)$v	$E(S_1)$	$E(T_1)$v	$E(T_1)$	$E(T_2)$	ΔE_{SF}	ΔE_{TTA}
Perylene	2.856	2.688	1.550	1.507	2.839	-0.326	-0.174
BP1	2.547	2.362	1.305	1.235	2.502	-0.109	0.032
BP2-a	2.376	2.161	1.187	1.095	2.101	-0.028	-0.088
BP2-b	2.409	2.064	1.223	1.029	2.411	0.005	0.352
BP2-Cs	2.389	2.166	1.178	1.069	2.227	0.028	0.090
BP3	2.300	1.978	1.154	0.975	2.071	0.027	0.121
BP4	2.243	1.925	1.147	0.971	1.973	-0.018	0.030
OP1	2.775	2.613	1.533	1.493	2.513	-0.372	-0.472
OP2-a	2.723	2.574	1.524	1.500	2.546	-0.427	-0.455
OP2-b	2.735	2.564	1.544	1.510	2.369	-0.456	-0.651
OP2-Cs	2.770	2.603	1.548	1.515	2.328	-0.428	-0.703
OP3	2.731	2.568	1.555	1.538	2.301	-0.508	-0.775
OP4	2.738	2.572	1.577	1.577	2.237	-0.583	-0.918
PP1	2.630	2.474	1.356	1.303	2.489	-0.133	-0.118
PP2-a	2.514	2.363	1.284	1.249	2.222	-0.136	-0.277
PP2-b	2.460	2.304	1.214	1.147	2.388	0.010	0.094
PP2-Cs	2.503	2.356	1.251	1.204	2.142	-0.053	-0.266
PP3	2.393	2.244	1.184	1.137	2.091	-0.031	-0.184
PP4	2.322	2.179	1.148	1.114	1.984	-0.049	-0.243

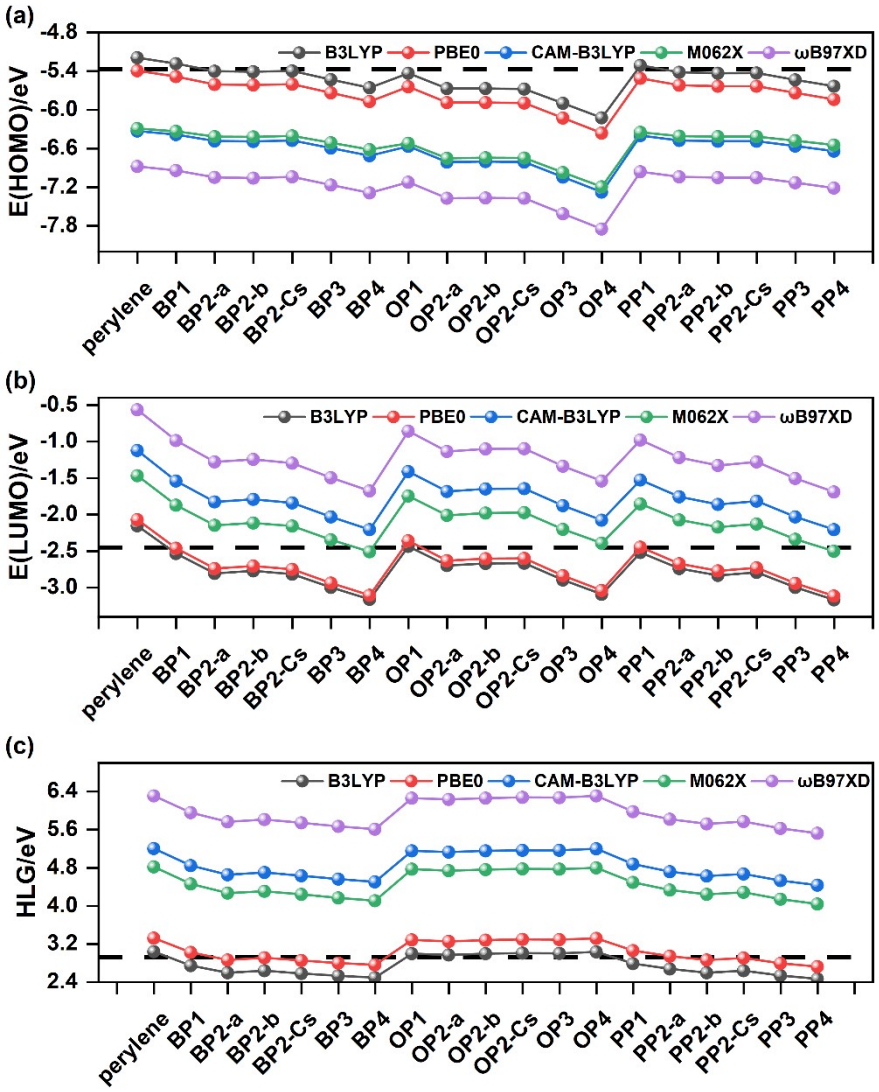

Fig. S1 Comparison of HOMO, LUMO energies and corresponding HLG using different exchange-correlation functionals (the dashed line represents the values estimated for perylene by the electrochemical method).

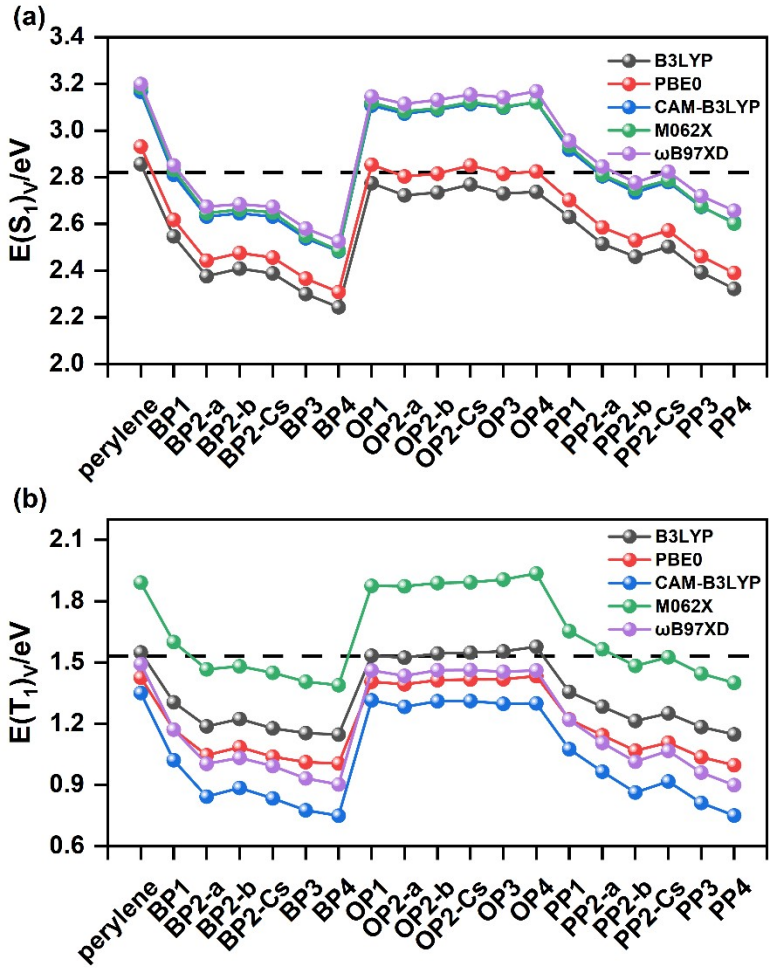

Fig. S2 Comparison of Vertical Excitation Energies $E(S_1)_V$ and $E(T_1)_V$ using different exchange-correlation functionalshe (dashed line indicates the experimental values for perylene).

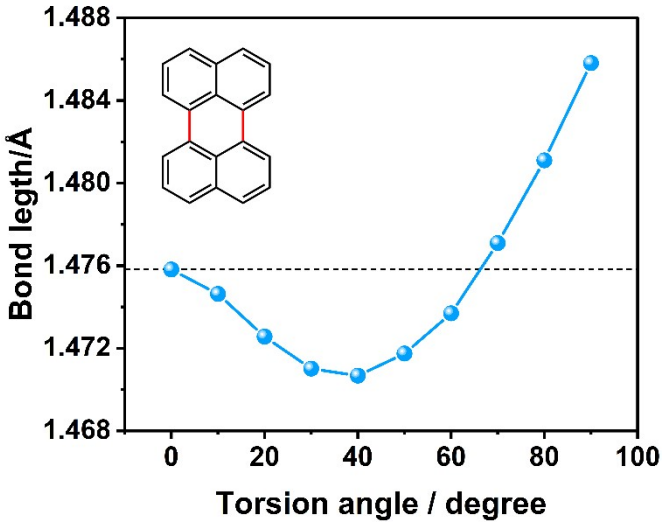

Fig. S3 Variation of the C-C σ-bond length between the two naphthalene fragments with the torsion angle (dashed line indicates the value when untwisted).

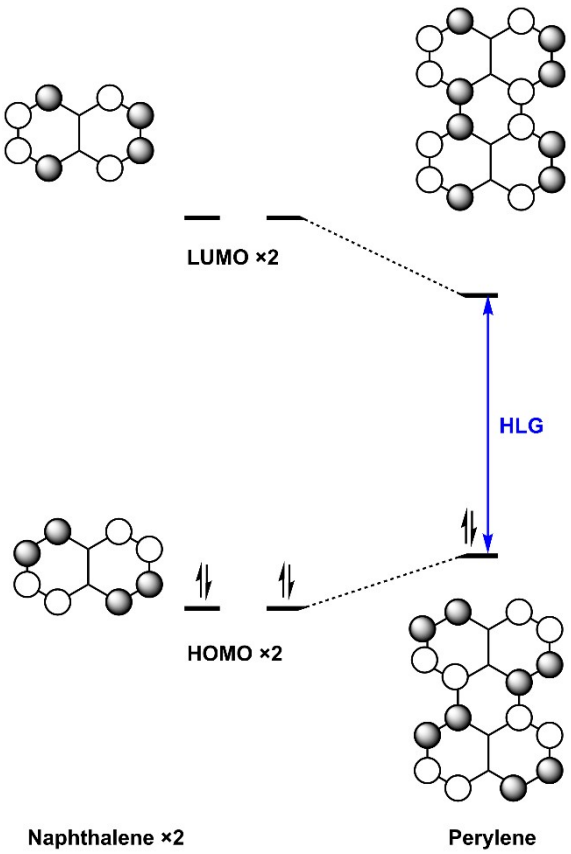

Fig. S4 Schematic diagram of the molecular orbital interaction of perylene. The parent MOs, that is, the HOMO and LUMO of naphthalene moieties, interact with each other and lead to the HOMO and LUMO orbital in perylene.

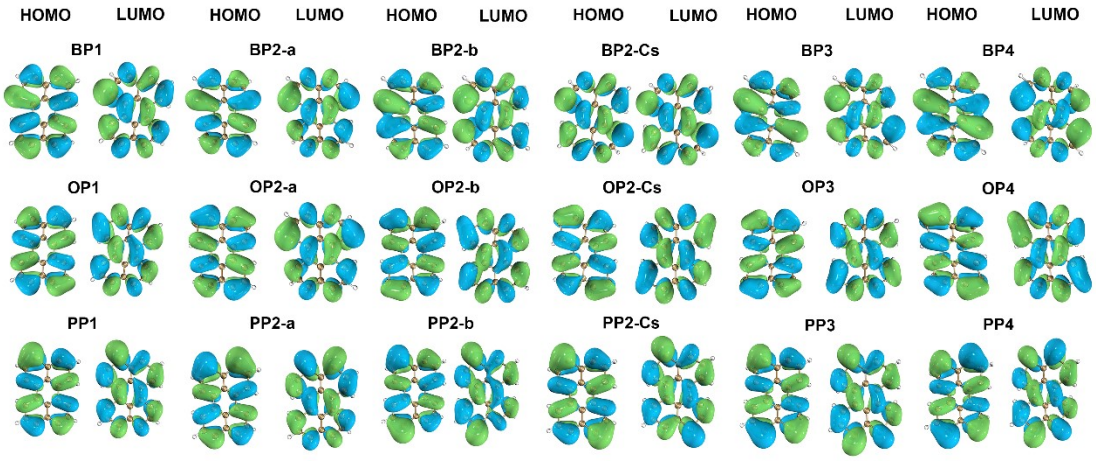

Fig. S5 HOMO and LUMO electron density distributions for mono phospha- and silcon-perylene derivatives based on B3LYP/6-311G* method. Drawn as isosurface of 0.02 e·bohr^{-3}.

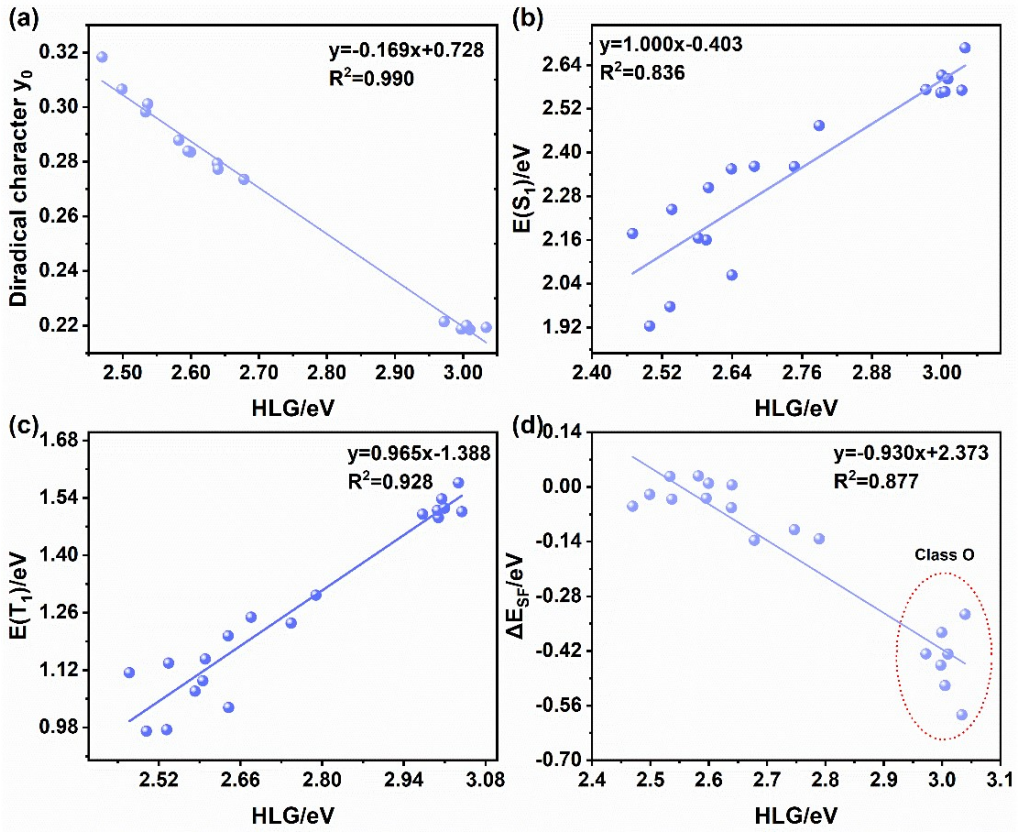

Fig. S6 Variation of diradical character y_0, $E(S_1)$, $E(T_1)$ and ΔE_{SF} of P-doped perylene as a function of HLG.

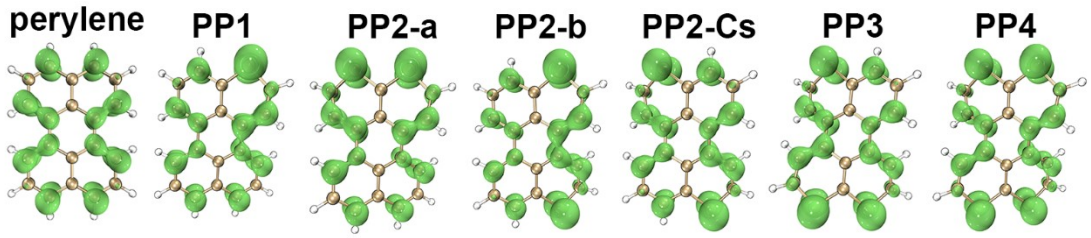

Fig. S7 The odd electron density Dodd y0(r) of P-doped perylene derivatives. The green surfaces represent the odd electron densities with the iso-surfaces with 0.002 e·bohr^{-3}.

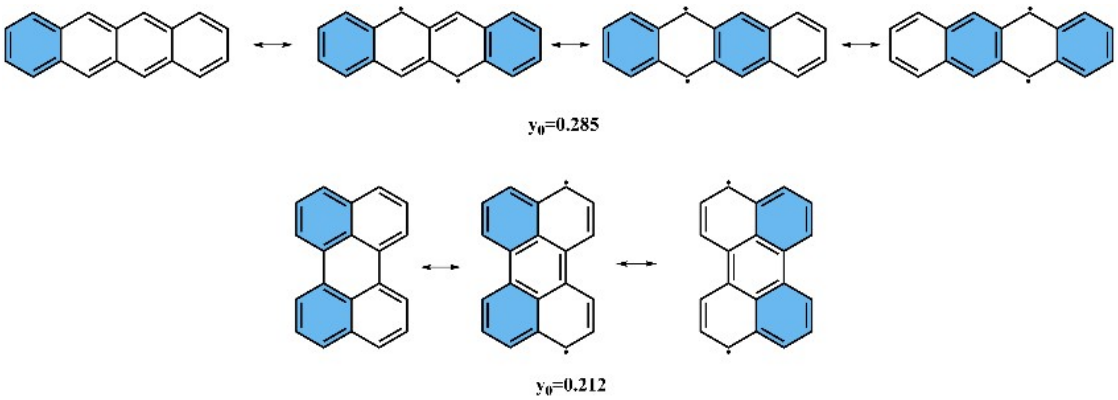

Fig. S8 The resonance structure of tetracene and perylene.

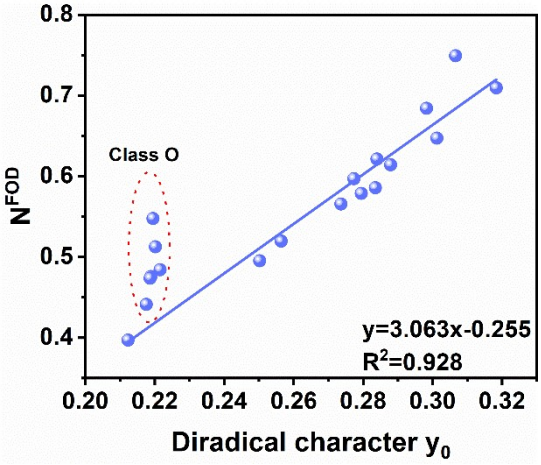

Fig. S9 Comparison of diradical character (y_0) and the N^{FOD} values for perylene derivatives.

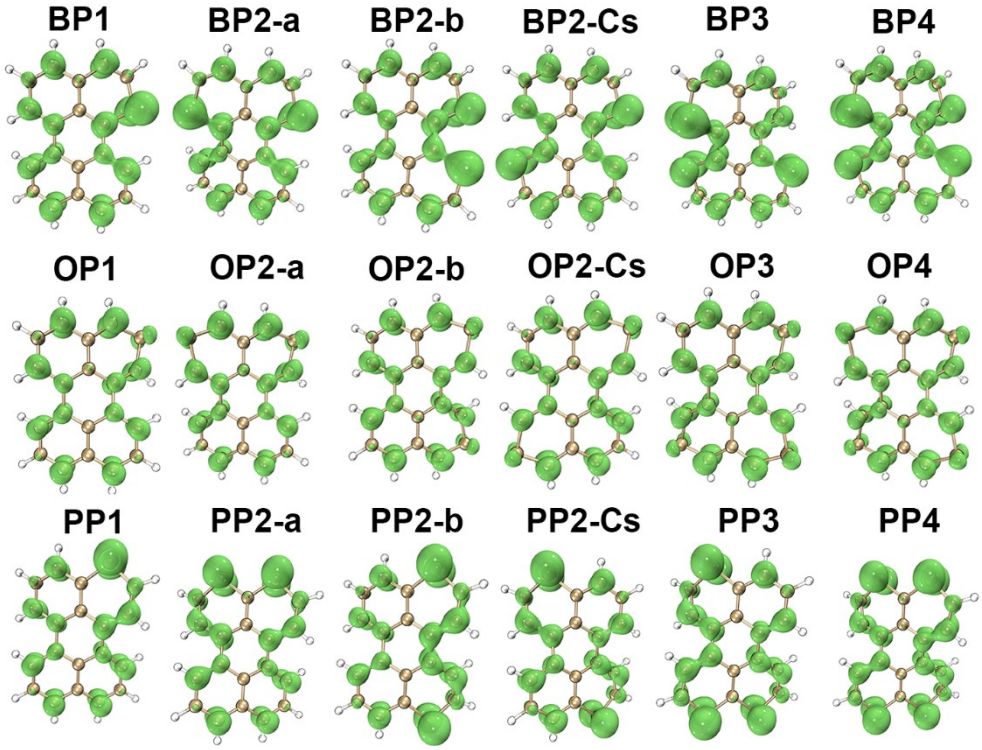

Fig. S10 Isocontour plot of the FOD density (isovalue =0.001 e·bohr^{-3}) calculated at FT-TPSS/def2-TZVP level.

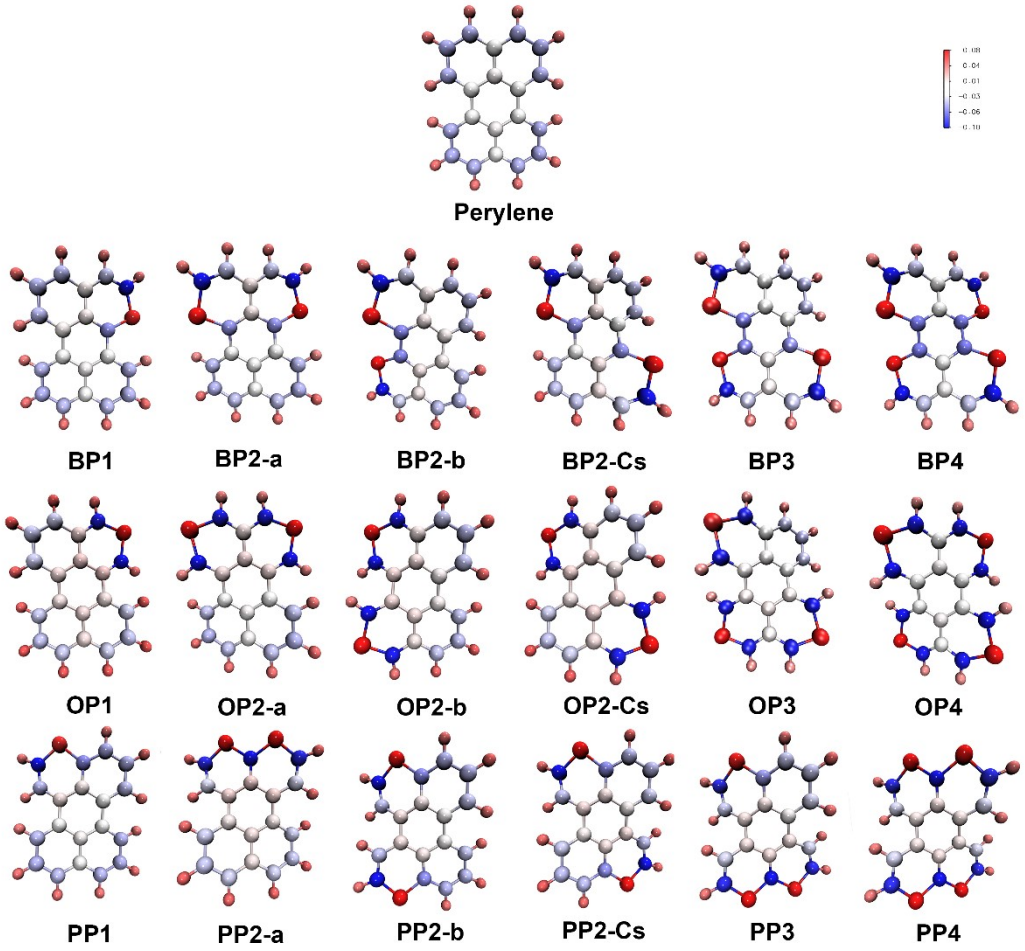

Fig. S11 Hirshfeld atomic charges of perylene derivatives.

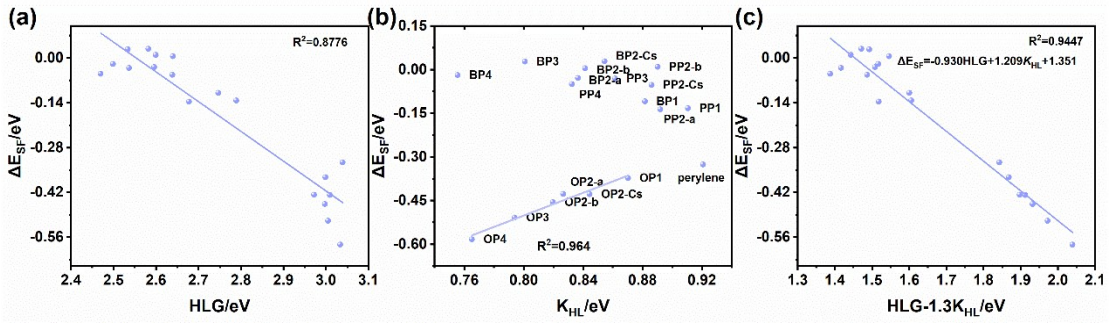

Fig. S12 The correlations between HLG, K_{HL}, HLG-1.3K_{HL} and the ΔE_{SF}.

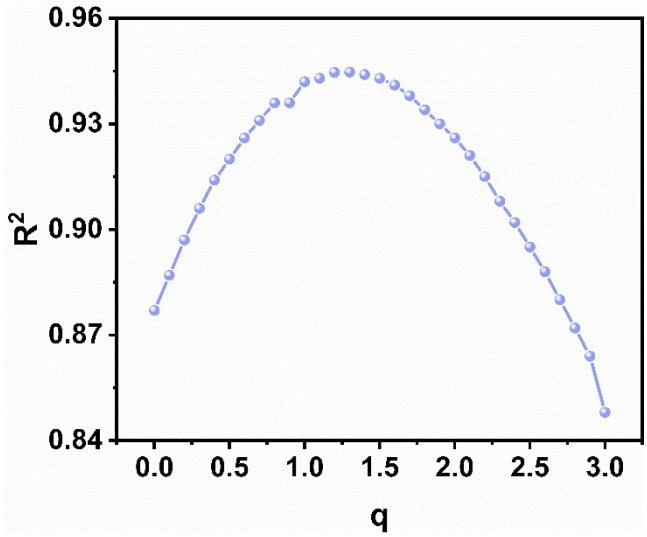

Fig. S13 The correlations between different ***q*** values and the R^2.

Coordinates of the computed molecules.

Perylene

C	-1.47819500	-2.42360600	-0.00037500
C	-0.73790700	-1.24819700	-0.00019000
C	-1.43851000	0.00000000	-0.00024500
C	-2.87249600	0.00000000	-0.00048900
C	-3.57130500	-1.23172400	-0.00067100
C	-2.88245200	-2.41902700	-0.00061400
H	-0.97760800	-3.38362200	-0.00033800
C	-0.73790700	1.24819700	-0.00006100
C	-3.57130500	1.23172500	-0.00054500
H	-4.65701700	-1.21972900	-0.00085600
H	-3.41706800	-3.36355600	-0.00075300
C	-2.88245200	2.41902700	-0.00036600
C	-1.47819500	2.42360600	-0.00012600
H	-4.65701700	1.21972900	-0.00073000
H	-3.41706800	3.36355600	-0.00040800
H	-0.97760800	3.38362200	0.00001000
C	2.88245200	-2.41902700	0.00036300
C	3.57130500	-1.23172500	0.00054300
C	2.87249600	0.00000000	0.00048900
C	1.43851000	0.00000000	0.00024500
C	0.73790700	-1.24819700	0.00006000
C	1.47819500	-2.42360600	0.00012300
H	4.65701700	1.21972900	0.00085700
H	3.41706800	-3.36355600	0.00040300
H	4.65701700	-1.21972900	0.00072900
C	3.57130500	1.23172400	0.00067300
C	0.73790700	1.24819700	0.00019100
H	0.97760800	-3.38362200	-0.00001400
C	1.47819500	2.42360600	0.00037800
C	2.88245200	2.41902700	0.00061700
H	0.97760800	3.38362200	0.00034200
H	3.41706800	3.36355600	0.00075700

BP1

C	0.74247200	-1.02022600	-0.02007900
C	1.31496600	0.29253700	0.02222400
C	2.73968500	0.49539300	0.04552300
C	3.66613300	-0.57633500	-0.06135300
C	3.31402100	-1.88616500	-0.21996400
C	0.46469700	1.45431000	0.05215400
C	3.25997500	1.80603600	0.17286600
H	4.72130300	-0.31252600	-0.03159400
H	4.09856100	-2.63007100	-0.33063600

C	2.42595600	2.89151000	0.26513800
C	1.03823000	2.71064700	0.19898200
H	4.33730600	1.93535400	0.20097900
H	2.83254700	3.89091800	0.38042900
H	0.40689900	3.58680800	0.27480000
C	-2.72562700	-2.54707100	0.31577800
C	-3.54305100	-1.45404400	0.15595700
C	-2.98402400	-0.16273700	0.00157800
C	-1.56000800	-0.00756500	0.00810000
C	-0.72331100	-1.16194900	0.10135200
C	-1.33043500	-2.40026300	0.29048600
H	-4.88432800	0.85422900	-0.17021200
H	-3.15242000	-3.53453900	0.45865400
H	-4.62320800	-1.56367900	0.15789400
C	-3.80599300	0.97977700	-0.15689000
C	-0.99480300	1.29882200	-0.07520600
H	-0.71789500	-3.28484200	0.41757000
C	-1.84767500	2.38132400	-0.25622400
C	-3.24276800	2.22394800	-0.30171500
H	-1.44633500	3.38025200	-0.37254500
H	-3.87160800	3.09707000	-0.44303500
P	1.66990300	-2.48844500	-0.25163700

BP2-a

C	0.52978000	1.24167000	0.02340400
C	1.25878200	-0.00010300	-0.00001000
C	2.70147400	-0.00018600	0.00016100
C	3.46164800	1.18779600	0.17639500
C	2.93917600	2.43392200	0.37680800
C	0.52960600	-1.24192600	-0.02354100
C	3.46155400	-1.18829100	-0.17604100
H	4.54307000	1.07162800	0.17028000
H	3.61825400	3.26388900	0.55243700
C	2.93891000	-2.43427700	-0.37672700
H	4.54299200	-1.07228800	-0.16951200
H	3.61782200	-3.26437800	-0.55229900
C	-3.05780400	2.35533000	-0.55819500
C	-3.75892100	1.20451700	-0.28402900
C	-3.07045600	0.00018400	0.00003700
C	-1.64009400	0.00007200	-0.00000800
C	-0.92969900	1.22059800	-0.18123700
C	-1.65475300	2.36434300	-0.50584500
H	-4.84471200	-1.20031600	0.29682700
H	-3.58474100	3.27034600	-0.80812700
H	-4.84453800	1.20096000	-0.29665200

C	-3.75909600	-1.20404500	0.28415500
C	-0.92989400	-1.22056400	0.18119900
H	-1.13426900	3.29088500	-0.71672000
C	-1.65509100	-2.36418100	0.50593600
C	-3.05814700	-2.35494700	0.55834700
H	-1.13472100	-3.29078700	0.71679600
H	-3.58521300	-3.26987100	0.80834500
P	1.23250600	2.81103800	0.35279400
P	1.23177300	-2.81100800	-0.35320900

BP2-b

C	-0.72743600	-0.93716100	0.10518200
C	-1.44896200	0.28962900	-0.03295000
C	-2.88227200	0.32431200	-0.09539300
C	-3.67516300	-0.83870800	0.10901400
C	-3.17061400	-2.06377900	0.44390300
C	-0.72651900	1.52472300	-0.11486500
C	-3.53414000	1.55366100	-0.35155900
H	-4.75334200	-0.71391800	0.03058400
H	-3.86449800	-2.87435400	0.65092600
C	-2.81573400	2.71390800	-0.51591700
C	-1.42060900	2.69839900	-0.38456200
H	-4.61763300	1.56410400	-0.41690600
H	-3.32362200	3.64806400	-0.73191500
H	-0.88182600	3.62980400	-0.50827000
C	3.17053100	-2.06381700	-0.44364300
C	3.67514200	-0.83874800	-0.10864700
C	2.88229300	0.32430500	0.09557400
C	1.44897500	0.28966000	0.03289900
C	0.72743000	-0.93717200	-0.10515900
H	4.61761900	1.56409400	0.41736500
H	3.86446300	-2.87437100	-0.65057500
H	4.75330100	-0.71411300	-0.02974500
C	3.53413800	1.55365800	0.35181700
C	0.72654000	1.52476100	0.11463200
C	1.42061800	2.69844800	0.38430400
C	2.81572400	2.71392500	0.51592000
H	0.88184900	3.62988300	0.50785100
H	3.32358800	3.64809000	0.73193700
P	-1.46242200	-2.45627100	0.58042400
P	1.46245200	-2.45621600	-0.58072700

BP2-Cs

C	-1.00297100	1.04135400	-0.04268600
C	-1.41517800	-0.32169300	0.05121400
C	-2.80279500	-0.69672400	0.07006800

C	-3.84564600	0.24636900	-0.13313700
C	-3.64417000	1.57366700	-0.38789700
C	-0.42415200	-1.35792800	0.15000000
C	-3.15628400	-2.04895500	0.29228400
H	-4.86325800	-0.13755300	-0.10312600
H	-4.50674800	2.20665300	-0.57850700
C	-2.19191800	-3.00829900	0.48323700
C	-0.83725300	-2.66122000	0.40927500
H	-4.20882000	-2.31280200	0.31998100
H	-2.47102200	-4.03764900	0.68228000
H	-0.09488400	-3.43675100	0.55477700
C	2.19174400	3.00828600	0.48343100
C	3.15615200	2.04901700	0.29230900
C	2.80275600	0.69676300	0.07002600
C	1.41518200	0.32160100	0.05126400
C	0.42413100	1.35779900	0.15009800
C	0.83710200	2.66110400	0.40952800
H	4.86326200	0.13787200	-0.10364300
H	2.47080000	4.03762900	0.68258100
H	4.20867300	2.31292600	0.31996700
C	3.84569400	-0.24618900	-0.13338600
C	1.00300800	-1.04145900	-0.04273900
H	0.09462900	3.43649700	0.55523700
C	3.64432400	-1.57349300	-0.38807900
H	4.50689800	-2.20644600	-0.57880600
P	-2.08293500	2.36963900	-0.41550800
P	2.08307600	-2.36966400	-0.41513200

BP3

C	-0.95584700	-0.95867300	0.13776600
C	-1.50750500	0.34072100	-0.05700800
C	-2.92182500	0.56875000	-0.10728700
C	-3.85814500	-0.46084700	0.18680300
C	-3.51406500	-1.72026400	0.59314800
C	-0.61769500	1.45005800	-0.22238600
C	-3.39923900	1.85595500	-0.44748600
H	-4.91162600	-0.19724600	0.11720000
H	-4.30548300	-2.41372900	0.86517300
C	-2.52616300	2.88611300	-0.71076100
C	-1.14504800	2.68537600	-0.58982800
H	-4.47138000	2.01599900	-0.50464100
H	-2.90120100	3.86239800	-0.99916900
H	-0.47800900	3.51677100	-0.78431600
C	2.68115400	-2.66115100	-0.55459400
C	3.37690000	-1.53395800	-0.21860700

C	2.79773700	-0.25688400	0.02348400
C	1.37449500	-0.04632700	-0.01361300
C	0.47338200	-1.16079900	-0.12270900
H	4.76140300	0.53458700	0.31983500
H	3.23647800	-3.56420700	-0.79364000
H	4.46227300	-1.58676100	-0.16770100
C	3.70659800	0.79910500	0.29617200
C	0.81930200	1.27453100	0.04702800
C	3.35048800	2.09573500	0.54814300
H	4.12941300	2.81201100	0.79511500
P	-1.87134200	-2.33694800	0.71680200
P	1.71702600	2.71563400	0.47598100
P	0.93238200	-2.77365200	-0.63128000
BP4			
C	0.71635000	1.21516300	0.15657600
C	1.45817800	-0.00001700	0.00001700
C	2.89434500	0.00000200	-0.00000300
C	3.64031600	1.16120300	0.33995600
C	3.09779300	2.35713100	0.72465400
C	0.71636500	-1.21523600	-0.15657300
C	3.64033900	-1.16119900	-0.33999900
H	4.72349400	1.06206700	0.32026900
H	3.76684400	3.15633000	1.03218800
C	3.09783500	-2.35712200	-0.72468300
H	4.72351600	-1.06203100	-0.32035500
H	3.76685800	-3.15633200	-1.03223500
C	-3.09784300	2.35712400	-0.72460400
C	-3.64035100	1.16116300	-0.33999300
C	-2.89435200	-0.00004100	-0.00007900
C	-1.45818500	-0.00003300	-0.00007200
C	-0.71635700	1.21516300	-0.15660400
H	-4.72349700	-1.06212500	0.32023800
H	-3.76688800	3.15635200	-1.03207000
H	-4.72352700	1.06200200	-0.32032300
C	-3.64031800	-1.16125100	0.33992800
C	-0.71636400	-1.21524000	0.15659200
C	-3.09777800	-2.35713800	0.72468100
H	-3.76678900	-3.15635600	1.03224400
P	1.38237800	2.72203400	0.75365900
P	-1.38228600	-2.72192800	0.75372800
P	-1.38239200	2.72200000	-0.75363800
P	1.38231100	-2.72196900	-0.75366400
OP1			
C	1.57502900	-2.07472100	-0.20416900

C	0.72314800	-0.99523400	-0.03106000
C	1.22414900	0.35197000	0.02751900
C	2.63794100	0.61972300	0.05754500
C	3.61458800	-0.40057900	-0.04197200
H	1.13375900	-3.05782500	-0.32027600
C	0.31456400	1.46107600	0.05454300
C	3.08687800	1.96159700	0.18899700
H	4.65309600	-0.08065300	-0.00410700
C	2.19621100	2.99938900	0.27603100
C	0.81918800	2.74673500	0.20265700
H	4.15551400	2.14728900	0.22339500
H	2.54874400	4.01907400	0.39277800
H	0.14289000	3.58883500	0.27388400
C	-2.66583800	-2.70347000	0.31182500
C	-3.53768700	-1.65548400	0.14896300
C	-3.04617100	-0.33716400	-0.00853700
C	-1.63193700	-0.10903000	-0.00152800
C	-0.73839800	-1.21915100	0.08903700
C	-1.27837600	-2.48491100	0.27848700
H	-4.99707400	0.57831800	-0.18339600
H	-3.04071600	-3.71106000	0.45933700
H	-4.61074000	-1.82063300	0.15157700
C	-3.92688300	0.76030200	-0.16838100
C	-1.13568300	1.22669000	-0.07913800
H	-0.62980300	-3.34045700	0.41633700
C	-2.04386600	2.26195300	-0.25934200
C	-3.42911100	2.03200700	-0.31002700
H	-1.69573000	3.28106400	-0.37123400
H	-4.10200000	2.87154400	-0.45155500
P	3.32637200	-2.07504600	-0.25169600

OP2-a

C	1.01303200	2.45904100	0.25977400
C	0.38815400	1.24256100	0.03401400
C	1.11868100	-0.00002700	0.00003400
C	2.56206200	-0.00006200	0.00006800
C	3.31816200	1.19362600	0.15598300
H	0.38449400	3.33555200	0.36685600
C	0.38808900	-1.24251700	-0.03405900
C	3.31803500	-1.19378400	-0.15577100
H	4.39848500	1.07626700	0.14772800
C	1.01287600	-2.45906300	-0.26001200
H	4.39837500	-1.07662900	-0.14734700
H	0.38415700	-3.33542300	-0.36734200
C	-3.20817900	2.35724300	-0.54194200

C	-3.90857400	1.20524300	-0.27852900
C	-3.21939100	0.00008500	0.00002800
C	-1.78844000	0.00006700	0.00001000
C	-1.08037700	1.22384200	-0.16518400
C	-1.80371400	2.36771600	-0.47625200
H	-4.99413200	-1.20051300	0.29358100
H	-3.73427500	3.27385700	-0.78761200
H	-4.99410500	1.20073100	-0.29348300
C	-3.90860200	-1.20505800	0.27860300
C	-1.08041700	-1.22373500	0.16517800
H	-1.29102800	3.29846300	-0.68443700
C	-1.80377200	-2.36759100	0.47627200
C	-3.20823700	-2.35707800	0.54200300
H	-1.29109000	-3.29834400	0.68445000
H	-3.73435500	-3.27367400	0.78769300
P	2.72749300	2.78103700	0.38968600
P	2.72698400	-2.78125900	-0.38978000

OP2-b

C	-1.39906800	-2.13520700	-0.37402800
C	-0.74019000	-0.95150700	-0.08674900
C	-1.45334100	0.28580900	0.04581700
C	-2.88889300	0.32081300	0.10612600
C	-3.68612300	-0.83493900	-0.07312900
H	-0.79912500	-3.01612400	-0.57305400
C	-0.72861300	1.51689800	0.11314000
C	-3.53730100	1.56221100	0.34710000
H	-4.76242300	-0.69661800	-0.00335400
C	-2.81527100	2.71773800	0.49949900
C	-1.41819700	2.69435700	0.37081700
H	-4.62046900	1.57596300	0.41180200
H	-3.31833300	3.65705900	0.70454200
H	-0.87763700	3.62519700	0.48704100
C	3.68611600	-0.83503700	0.07336600
C	2.88897000	0.32074200	-0.10601800
C	1.45339400	0.28576700	-0.04597100
C	0.74029200	-0.95151500	0.08652200
C	1.39916600	-2.13531200	0.37374600
H	4.62060400	1.57592200	-0.41136100
H	4.76243400	-0.69679500	0.00388800
C	3.53742500	1.56216900	-0.34685400
C	0.72868900	1.51688900	-0.11332800
H	0.79912300	-3.01617000	0.57269800
C	1.41831000	2.69431700	-0.37095200
C	2.81542200	2.71767900	-0.49941900

H	0.87778700	3.62517200	-0.48724300
H	3.31851500	3.65699500	-0.70441100
P	-3.13031700	-2.41328500	-0.44167400
P	3.12997000	-2.41350400	0.44176400
OP2-Cs			
C	2.03051600	-1.93022200	0.33980200
C	1.06407700	-0.97785200	0.06120500
C	1.39394200	0.41337800	-0.04851500
C	2.76035700	0.85812800	-0.07780300
C	3.85219500	-0.02191700	0.11580200
H	1.70721300	-2.95192100	0.50487000
C	0.34747100	1.38500300	-0.13699100
C	3.03096500	2.23364700	-0.30963200
H	4.84441200	0.42100700	0.07528900
C	2.01195100	3.13197900	-0.49365400
C	0.67768300	2.70842300	-0.39778800
H	4.06592200	2.55773400	-0.34864000
H	2.22872500	4.17495300	-0.69992700
H	-0.10402700	3.44238000	-0.54572900
C	-2.01196200	-3.13199200	-0.49370100
C	-3.03097800	-2.23371100	-0.30942800
C	-2.76037400	-0.85816500	-0.07772500
C	-1.39395500	-0.41340200	-0.04848500
C	-0.34749000	-1.38500300	-0.13707400
C	-0.67769900	-2.70838600	-0.39806100
H	-4.84443400	-0.42103800	0.07540800
H	-2.22873000	-4.17495700	-0.70002500
H	-4.06592900	-2.55783400	-0.34827200
C	-3.85220700	0.02186000	0.11588000
C	-1.06410100	0.97783000	0.06131500
H	0.10400700	-3.44227800	-0.54634500
C	-2.03059600	1.93024600	0.33960500
H	-1.70728600	2.95198700	0.50440600
P	3.76633700	-1.70069000	0.44671800
P	-3.76624700	1.70075100	0.44664500
OP3			
C	1.88014000	-1.98078100	-0.51630700
C	1.05894200	-0.93550800	-0.13111200
C	1.57391300	0.38375800	0.06756900
C	2.98488400	0.64119500	0.12508000
C	3.94673900	-0.35865000	-0.15418800
H	1.41662300	-2.93065900	-0.75981200
C	0.66137100	1.47037600	0.21352100
C	3.42672900	1.94695300	0.47022400

H	4.99044300	-0.06141800	-0.08503200
C	2.52782800	2.95122900	0.72455100
C	1.15070300	2.71636100	0.58115300
H	4.49393700	2.13207600	0.53709000
H	2.87414800	3.93669400	1.01793200
H	0.46579700	3.53225600	0.77513600
C	-3.29171000	-1.58770200	0.20651300
C	-2.73433900	-0.29995700	-0.01877300
C	-1.31144900	-0.07238600	0.00558000
C	-0.39280200	-1.17355200	0.10465800
C	-0.81177000	-2.45551600	0.41880200
H	-4.70804800	0.47004900	-0.27681900
H	-4.37629700	-1.64938200	0.17434400
C	-3.65831800	0.75119900	-0.26640900
C	-0.77956700	1.26123300	-0.06265100
H	-0.04923200	-3.20753400	0.58769300
C	-1.56929300	2.35529800	-0.37563700
H	-1.07737000	3.31271200	-0.50586000
P	3.63243400	-1.97269300	-0.64015900
P	-3.30819500	2.39582400	-0.58208900
P	-2.45770600	-3.03753700	0.56757300

OP4

C	1.32782500	2.39725400	0.56254200
C	0.72897900	1.21878400	0.15331200
C	1.46770300	0.00004500	-0.00003900
C	2.90684100	0.00005000	0.00002900
C	3.65113300	1.16430300	0.33093200
H	0.68563400	3.24845400	0.76089000
C	0.72904400	-1.21874300	-0.15336600
C	3.65121400	-1.16415000	-0.33081400
H	4.73283500	1.05925700	0.31727600
C	1.32800800	-2.39720400	-0.56246200
H	4.73290700	-1.05904500	-0.31707400
H	0.68587800	-3.24844600	-0.76082100
C	-3.65119500	1.16438000	-0.33032100
C	-2.90686500	0.00003400	0.00023600
C	-1.46771400	-0.00000400	0.00012300
C	-0.72906100	1.21874700	-0.15344000
C	-1.32794800	2.39708700	-0.56299400
H	-4.73288300	-1.05925000	0.31712400
H	-4.73289700	1.05943000	-0.31616600
C	-3.65118400	-1.16426000	0.33084600
C	-0.72903700	-1.21875200	0.15333900
H	-0.68575500	3.24818300	-0.76178300

C	-1.32794500	-2.39727600	0.56240900
H	-0.68576100	-3.24846800	0.76078500
P	3.04143800	2.69754400	0.78792000
P	-3.04141900	-2.69765200	0.78771600
P	-3.04155800	2.69743500	-0.78793100
P	3.04162200	-2.69745400	-0.78785400
PP1			
C	-1.40952200	-2.23629700	-0.22229400
C	-0.62314400	-1.10025200	-0.04482700
C	-1.21233400	0.20906700	0.01695200
C	-2.63596800	0.38842200	0.04230300
C	-2.80492800	-2.26743500	-0.27127000
H	-0.90628700	-3.18833800	-0.34368800
C	-0.37265500	1.37391000	0.05557900
C	-3.17120900	1.69129800	0.17831600
H	-3.27653100	-3.23591800	-0.41686700
C	-2.34844600	2.78746200	0.27926600
C	-0.96028900	2.62345300	0.21118500
H	-4.25000800	1.81366600	0.20644100
H	-2.76731200	3.78096100	0.40223400
H	-0.33896100	3.50642200	0.29135000
C	2.86016000	-2.59985100	0.28853600
C	3.66540400	-1.49781100	0.13722000
C	3.09268100	-0.21133000	-0.00895900
C	1.66699500	-0.07153900	-0.00410300
C	0.84242700	-1.23656400	0.07458400
C	1.46248900	-2.46889400	0.25523700
H	4.98355400	0.82480200	-0.16802700
H	3.29732900	-3.58323800	0.42802500
H	4.74663700	-1.59565700	0.14102400
C	3.90412500	0.94006400	-0.15511500
C	1.08913800	1.23141400	-0.07226900
H	0.87058300	-3.36544300	0.38623600
C	1.93232400	2.32325300	-0.23917700
C	3.32886500	2.18001800	-0.28610900
H	1.52165600	3.31965900	-0.34305500
H	3.94907600	3.06089700	-0.41682900
P	-3.84442700	-0.91254200	-0.10514500
PP2-a			
C	-0.94163000	2.45537400	0.30197000
C	-0.30810500	1.23971900	0.05407300
C	-1.04218800	-0.00000700	0.00002000
C	-2.47627200	-0.00000200	0.00000200
C	-2.31633500	2.65303800	0.42325500

H	-0.31445700	3.33072600	0.42768100
C	-0.30809900	-1.23973000	-0.05402500
H	-2.66476700	3.66121600	0.63186700
C	-2.31633200	-2.65305500	-0.42319000
C	-0.94162300	-2.45538900	-0.30191000
H	-2.66477100	-3.66124000	-0.63176100
H	-0.31445600	-3.33075400	-0.42755300
C	3.28456200	2.37008100	-0.48458400
C	3.98415300	1.21137600	-0.24804500
C	3.29397400	0.00000900	-0.00000900
C	1.86301100	0.00000200	0.00000500
C	1.15424200	1.22870700	-0.13901400
C	1.88088600	2.38027200	-0.42338400
H	5.06967900	-1.20648200	0.26161500
H	3.81207900	3.29180600	-0.70739000
H	5.06966200	1.20651700	-0.26166800
C	3.98417000	-1.21135100	0.24801300
C	1.15425400	-1.22870900	0.13903400
H	1.37044200	3.31597200	-0.61376700
C	1.88091700	-2.38026900	0.42337700
C	3.28459400	-2.37006500	0.48455500
H	1.37049100	-3.31598000	0.61375400
H	3.81212300	-3.29178700	0.70734400
P	-3.50770800	1.43184400	0.23833600
P	-3.50769800	-1.43184300	-0.23840200

PP2-b

C	1.39642400	-2.25718400	0.37151400
C	0.73268600	-1.06378800	0.08840700
C	1.45371500	0.17092600	-0.02837300
C	2.88591800	0.20717300	-0.07396000
C	2.78197900	-2.42053100	0.44292400
H	0.79677600	-3.13842600	0.56792900
C	0.72921000	1.40382500	-0.10293900
C	3.53917000	1.44194500	-0.30027800
H	3.15438100	-3.41438500	0.67736300
C	2.82051600	2.60308300	-0.46267800
C	1.42487300	2.58081500	-0.35260600
H	4.62394900	1.45997700	-0.34882200
H	3.32896400	3.54093400	-0.66105800
H	0.88585300	3.51192800	-0.47579600
C	-2.78193500	-2.42057800	-0.44282300
C	-2.88592300	0.20712500	0.07395500
C	-1.45373000	0.17089700	0.02840400
C	-0.73268100	-1.06380200	-0.08834000

C	-1.39639700	-2.25721200	-0.37142900
H	-4.62399000	1.45989200	0.34877600
H	-3.15434200	-3.41444400	-0.67720500
C	-3.53920900	1.44188100	0.30026200
C	-0.72924900	1.40381000	0.10298300
H	-0.79673300	-3.13847300	-0.56771100
C	-1.42493500	2.58078600	0.35264600
C	-2.82058200	2.60303000	0.46269700
H	-0.88593200	3.51190800	0.47584600
H	-3.32905000	3.54086900	0.66107500
P	3.95480300	-1.19709800	0.16769400
P	-3.95473500	-1.19710200	-0.16786700

PP2-Cs

C	-1.77643000	-2.17431200	-0.34495000
C	-0.92972700	-1.10103900	-0.07663000
C	-1.43474000	0.23552700	0.02517800
C	-2.84171400	0.50796100	0.05129000
C	-3.16897000	-2.10764700	-0.43619200
H	-1.32757800	-3.14743100	-0.50886000
C	-0.51422200	1.33192500	0.11357700
C	-3.28510100	1.83297700	0.27439900
H	-3.69842000	-3.03043700	-0.65884700
C	-2.38659300	2.85692000	0.46233700
C	-1.01259000	2.60477200	0.37317900
H	-4.35256000	2.03030300	0.30688900
H	-2.73525100	3.86381500	0.66718200
H	-0.33123500	3.43217200	0.52518900
C	2.38660200	-2.85690800	0.46238100
C	3.28510500	-1.83296900	0.27437900
C	2.84169700	-0.50796500	0.05128900
C	1.43475500	-0.23550400	0.02520000
C	0.51424200	-1.33190300	0.11364100
C	1.01259500	-2.60474800	0.37326400
H	2.73526500	-3.86380100	0.66722800
H	4.35256500	-2.03029500	0.30682800
C	0.92975600	1.10104100	-0.07664600
H	0.33122100	-3.43213100	0.52528200
C	1.77648000	2.17430800	-0.34491500
C	3.16898600	2.10766200	-0.43603600
H	1.32765500	3.14744800	-0.50875600
H	3.69849000	3.03044600	-0.65858800
P	-4.12568700	-0.70174000	-0.19902400
P	4.12562500	0.70169500	-0.19911100

PP3

C	-1.75485000	-2.19437700	-0.49250300
C	-1.01404300	-1.07022000	-0.13056900
C	-1.64140700	0.20460300	0.03650600
C	-3.06518200	0.34906700	0.08072200
C	-3.14747500	-2.24327300	-0.59986100
H	-1.21616500	-3.10664700	-0.72354000
C	-0.81904500	1.36699400	0.17287200
C	-3.61734700	1.61437500	0.39172200
H	-3.59065300	-3.18859100	-0.90198300
C	-2.80657200	2.69792800	0.63994000
C	-1.41672300	2.57488600	0.51741500
H	-4.69720300	1.71790600	0.44209800
H	-3.23815200	3.65504700	0.91364700
H	-0.80409200	3.44706100	0.70916000
C	2.32545800	-2.72750700	0.56934300
C	2.69815400	-0.12664500	-0.01207100
C	1.27019900	-0.01522400	0.00219300
C	0.43774800	-1.18523600	0.10205100
C	0.96987500	-2.43207300	0.42894800
H	2.59407300	-3.74350900	0.84638700
C	0.62943800	1.26874200	-0.08037900
H	0.27383700	-3.24376100	0.60880300
C	1.34024500	2.42371000	-0.39878400
C	2.72246800	2.50821400	-0.56497500
H	0.77448300	3.33695300	-0.54723400
H	3.14025900	3.47503900	-0.83320000
P	-4.23113600	-0.95377800	-0.26134800
P	3.82629300	1.21252200	-0.33958100
P	3.61137400	-1.62096300	0.30162600

PP4

C	-1.33621200	2.40639600	0.54212900
C	-0.72303500	1.21989500	0.14322600
C	-1.46626300	-0.00003800	0.00002300
C	-2.89700200	0.00000600	0.00002200
C	-2.70779500	2.58656900	0.72342500
H	-0.69780300	3.25902300	0.74708200
C	-0.72306000	-1.21997500	-0.14324600
H	-3.04796300	3.56193500	1.06115100
C	-2.70791200	-2.58656300	-0.72342100
C	-1.33633000	-2.40644100	-0.54215500
H	-3.04812600	-3.56190500	-1.06116800
H	-0.69799200	-3.25910500	-0.74716100
C	2.70782400	2.58652400	-0.72350900
C	2.89700100	0.00000900	0.00000600

C	1.46626500	-0.00003400	-0.00001200
C	0.72304200	1.21989400	-0.14323400
C	1.33623100	2.40637100	-0.54218600
H	3.04797600	3.56187600	-1.06129600
C	0.72304300	-1.21999000	0.14313600
H	0.69782700	3.25897500	-0.74724800
C	1.33631300	-2.40648400	0.54190000
C	2.70791600	-2.58659400	0.72322900
H	0.69799000	-3.25918100	0.74681200
H	3.04809500	-3.56197800	1.06089600
P	-3.91325500	1.40307700	0.41005400
P	3.91334300	-1.40300100	0.41024500
P	3.91330300	1.40309300	-0.41003200
P	-3.91340200	-1.40296300	-0.40993900

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