Electronic Supplementary Information (ESI) for New Journal of Chemistry.

"Hot exciton" Fluorescence and Charge Transport of Fine-Tuned Twistacenes: Theoretical Study on Substitution Effect and Intermolecular Interactions

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Computational Details.

(R)ISC Rates. For the S1 and T2 states, λ could be formulated as,

$$\begin{aligned}\lambda_S &= E_{S1}(\mathrm{T2-geometry}) - E_{S1}(\mathrm{S1\text{-}geometry}) \\ \lambda_T &= E_{T2}(\mathrm{S1-geometry}) - E_{T2}(\mathrm{T2\text{-}geometry})\end{aligned} \tag{1}$$

where E_{S1}(T2/S1-geometry) is the S1 energy at T2/S1 minimum geometry, and E_{T2}(S1/T2-geometry) is the T2 energy at S1/T2 minimum geometry.

Carrier Mobility. Based upon Koopmans' theorem, V can be obtained by the energy splitting of the frontier or near-frontier molecular orbitals. Thus, intramolecular and inter-molecular electronic couplings V for hole and electron are calculated from energies as follows,

$$\begin{aligned}V_h &= \frac{(E_{\mathrm{HOMO}} - E_{\mathrm{HOMO\text{-}1}})}{2} \\ V_e &= \frac{(E_{\mathrm{LUMO+1}} - E_{\mathrm{LUMO}})}{2}\end{aligned} \tag{2}$$

where E_{HOMO}, $E_{\mathrm{HOMO\text{-}1}}$, E_{LUMO} and $E_{\mathrm{LUMO+1}}$ is the energy of HOMO, the nearest doubly occupied molecular orbital below HOMO, LUMO and the nearest unoccupied molecular orbital above LUMO for the molecules or their dimers, respectively. Meanwhile, λ is calculated from electronic energies as follows:

$$\begin{aligned}\lambda_h &= E(\mathrm{Ar}^+ / \mathrm{Ar}) - E(\mathrm{Ar}^+ / \mathrm{Ar}^+) + E(\mathrm{Ar} / \mathrm{Ar}^+) - E(\mathrm{Ar} / \mathrm{Ar}) \\ \lambda_e &= E(\mathrm{Ar}^- / \mathrm{Ar}) - E(\mathrm{Ar}^- / \mathrm{Ar}^-) + E(\mathrm{Ar} / \mathrm{Ar}^-) - E(\mathrm{Ar} / \mathrm{Ar})\end{aligned} \tag{3}$$

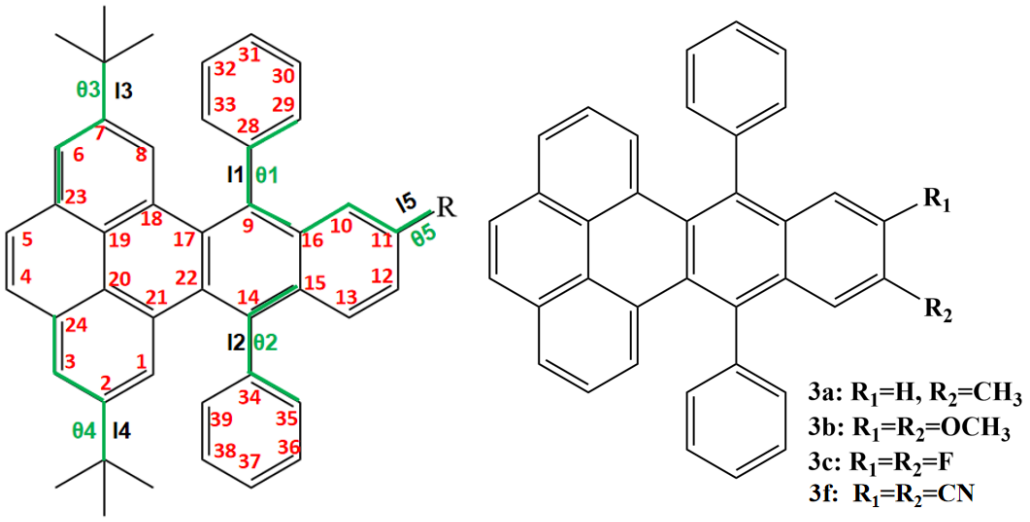
where Ar, Ar+ and Ar^- represent the molecules or species with neutral, +1 and -1 charges, and $E(Ar^+/Ar)$, $E(Ar^+/Ar^+)$, $E(Ar/Ar^+)$, $E(Ar^-/Ar)$, $E(Ar^-/Ar^-)$, $E(Ar/Ar^-)$, and $E(Ar/Ar)$ represent the single point energy of the cationic molecule with the optimized neutral geometry, the energy of the optimized cationic geometry, the single point energy of the neutral molecule with the optimized cationic geometry, the single point energy of anionic molecule with the neutral geometry, the energy of optimized anionic geometry, the single point energy of neutral molecule with the anionic geometry, and the energy of the optimized neutral geometry, respectively.

The charge carrier mobility is obtained according to the Einstein equation, and is expressed as,

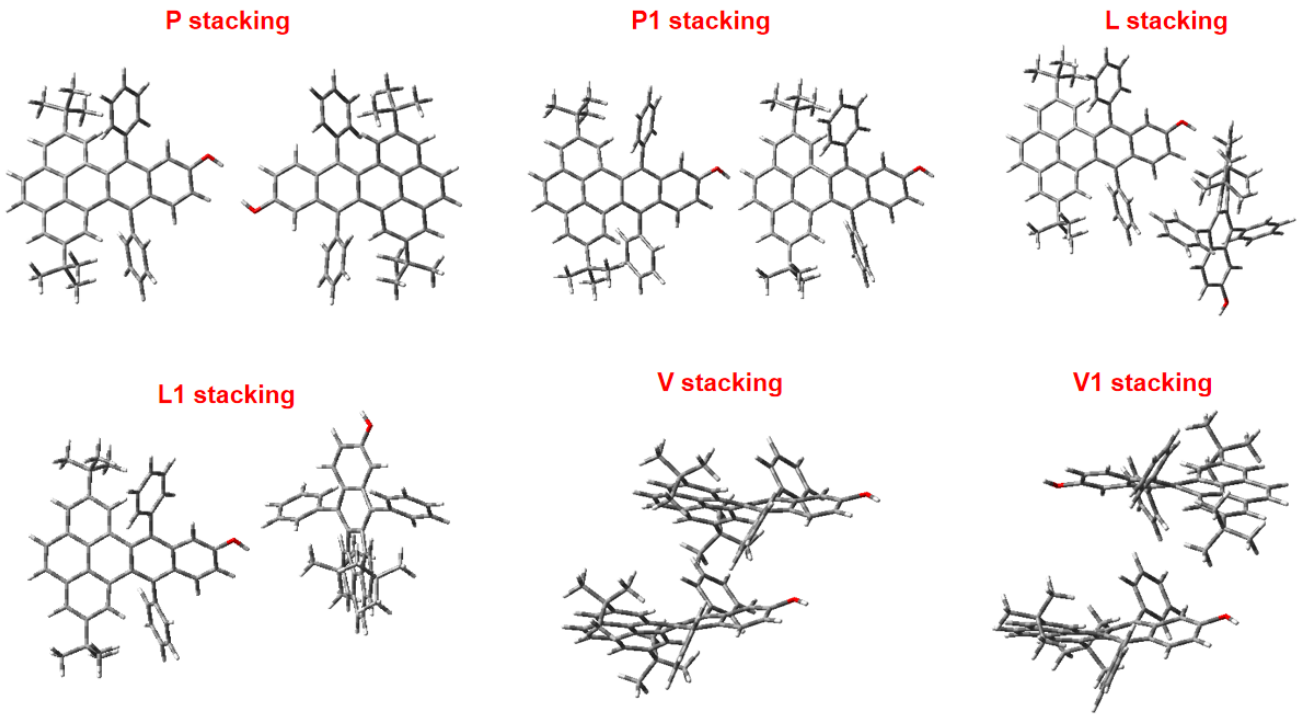
$$\mu = \frac{eD}{k_B T} \tag{4}$$

$$D = \frac{r^2 k}{2} \tag{5}$$

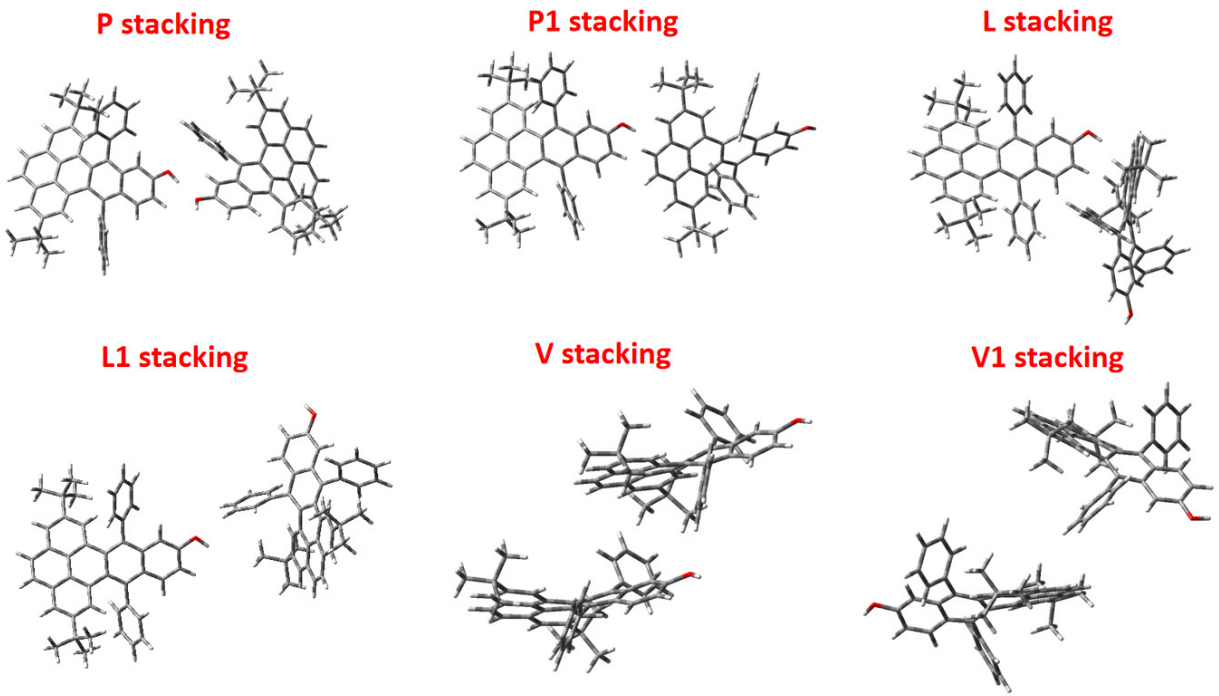
In which e is the charge of an electron, D is the diffusion parameter, r is the intramolecular distance from the centre of mass of benzo[f]tetraphene to the substituents for monomers or intermolecular CM distance (or benzene ring and substituent group or two benzene rings) between two neighbouring molecules.



Scheme S1. Chemical structures of (a) 1-H and its one substituent replaced derivatives at 11-position (R=H, CH_3, OH, OCH_3, NH_2, F, CN, NO_2) and (b) 3a, 3b, 3c and 3f in Ref. [*Dyes Pigments* 2015, **112**, 176-182].



Scheme S2. The un-optimized initial conformation of dimers.



Scheme S3. Molecular stacking patterns, where the two molecules with the substituents arranged in a head-to-head parallel was designated as P stacking, the substituents displaced in a head-to-tail parallel as P1, the benzo[f]tetraphene frame arranged in herringbone way as L, benzo[f]tetraphene arranged in L shape as L1 and benzo[f]tetraphene displaced vertically as V, pyrene units arranged vertically as V1, respectively. All of these dimers were optimized at B3LYP/6-311G** level.

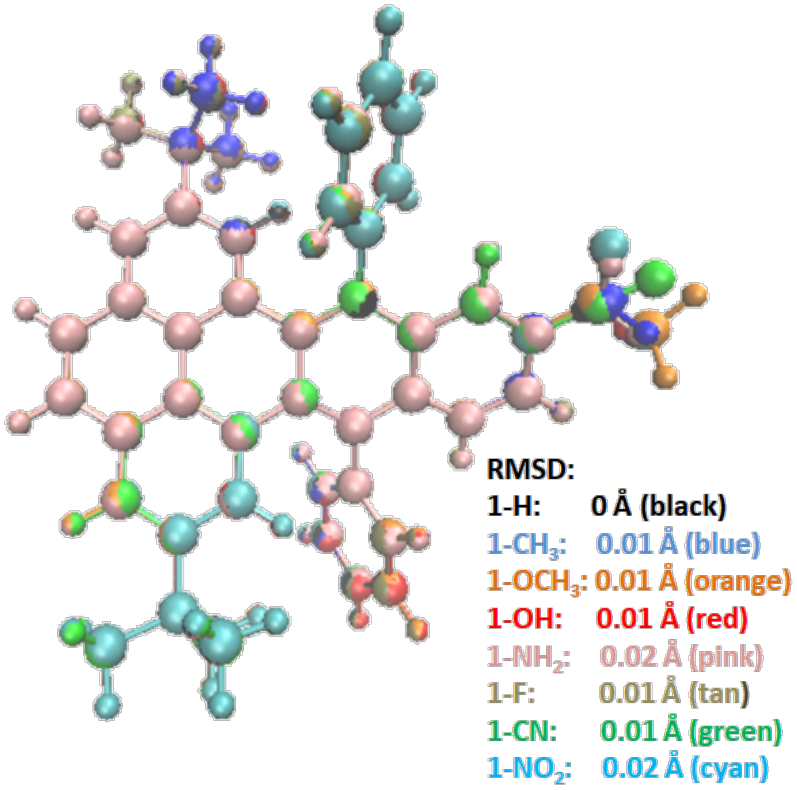


Figure S1. Intuitive picture of comparing the ground state geometries for 1-H and its derivatives. The root mean square displacement (RMSD) is listed on the right. (Black, blue, orange, red, pink, tan, green and cyan represent 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2, repectively.)

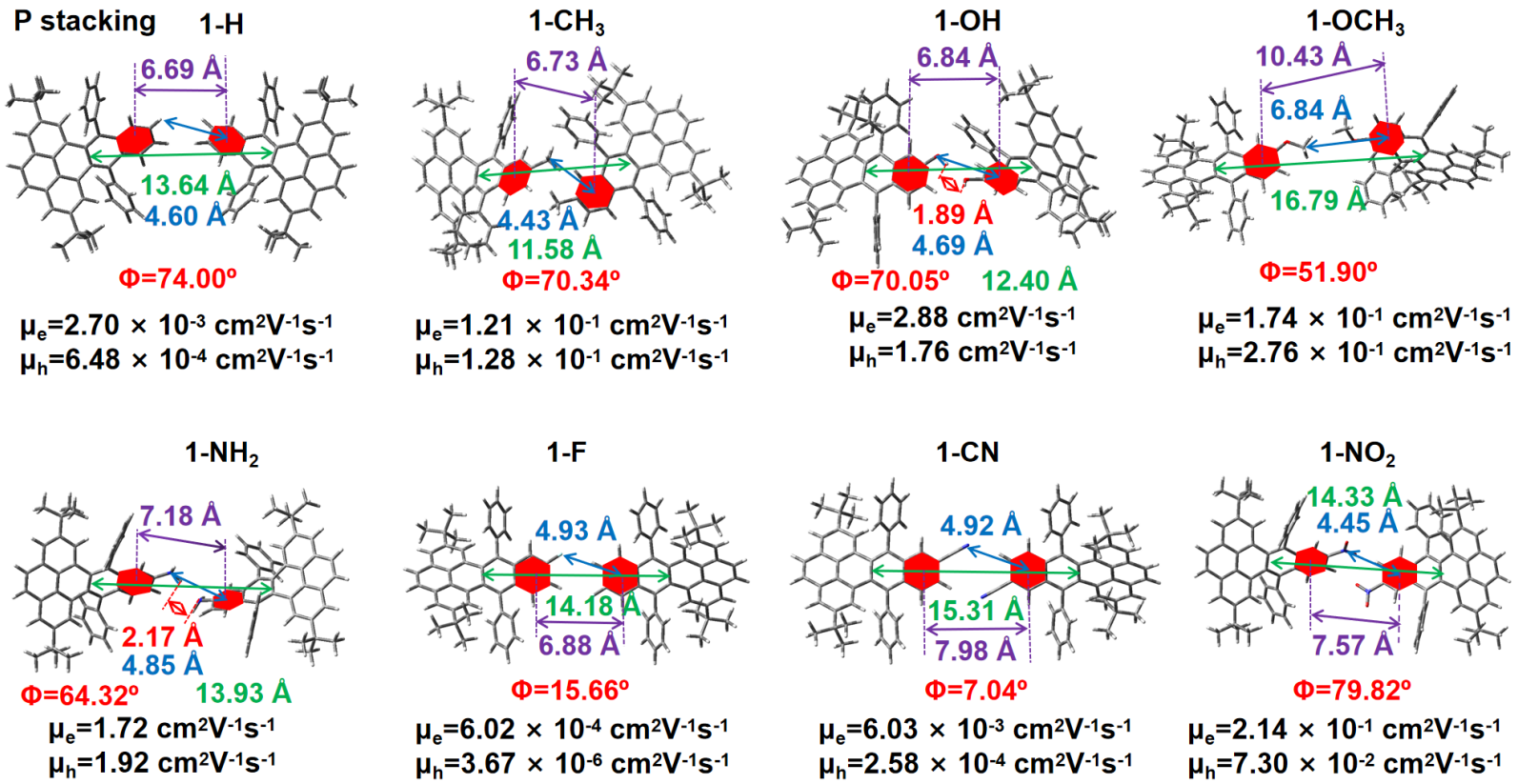


Figure S2. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives along P stacking mode, where Φ is the twisted angle of two benzene rings.

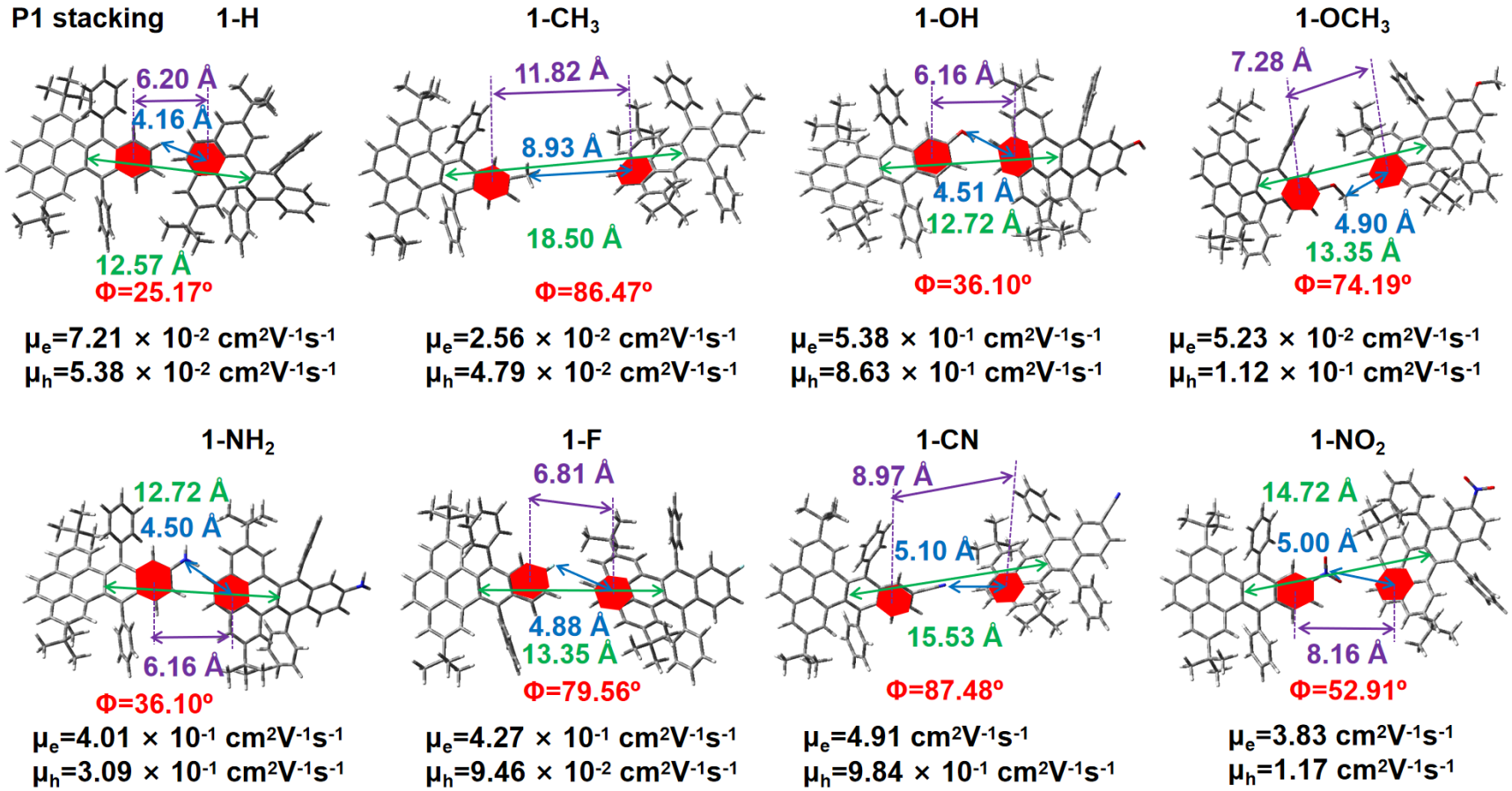


Figure S3. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives in P1 stacking mode, where Φ is the twisted angle of two benzene rings.

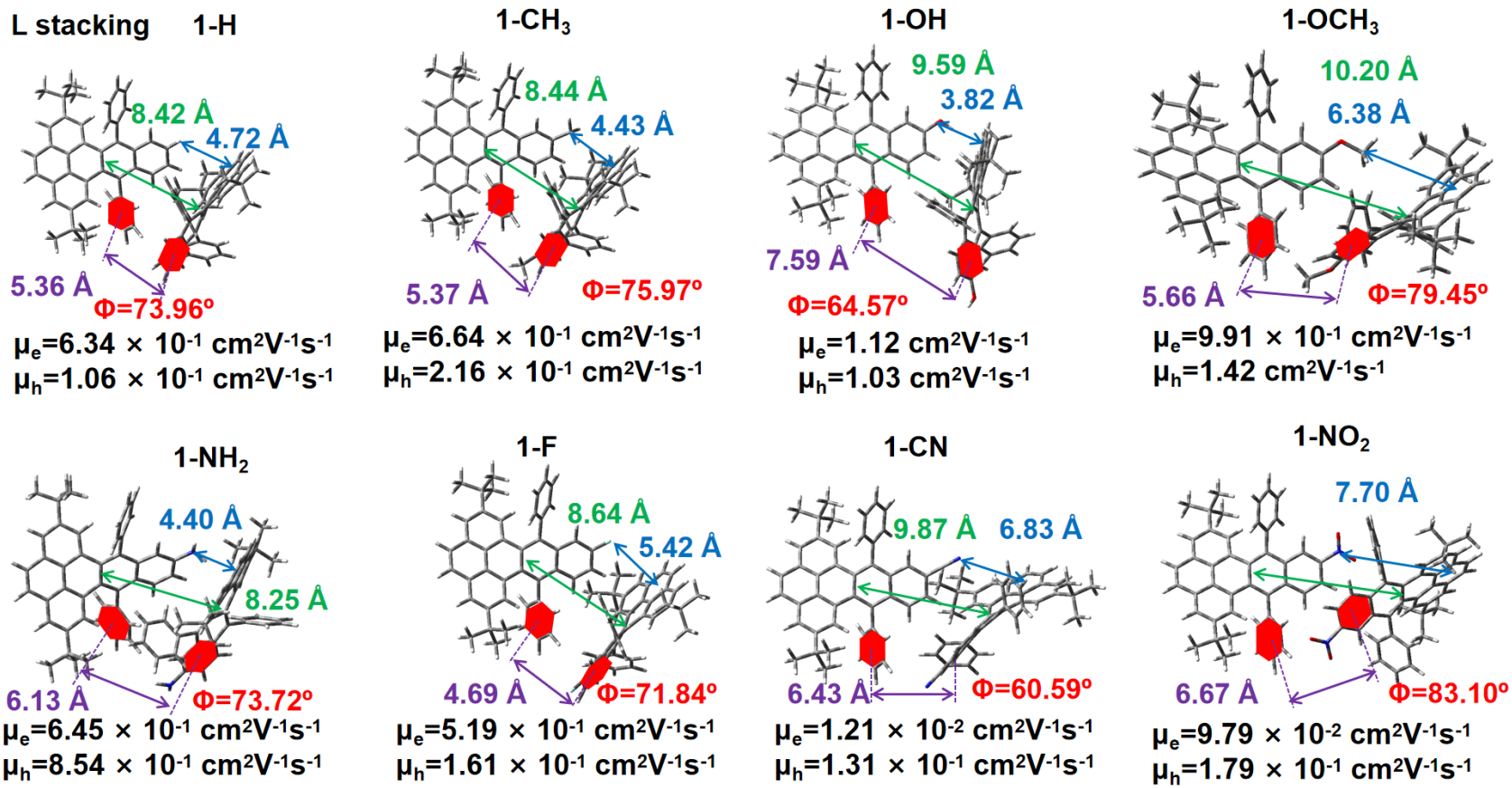


Figure S4. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives in L stacking mode, where Φ is the twisted angle of two benzene rings.

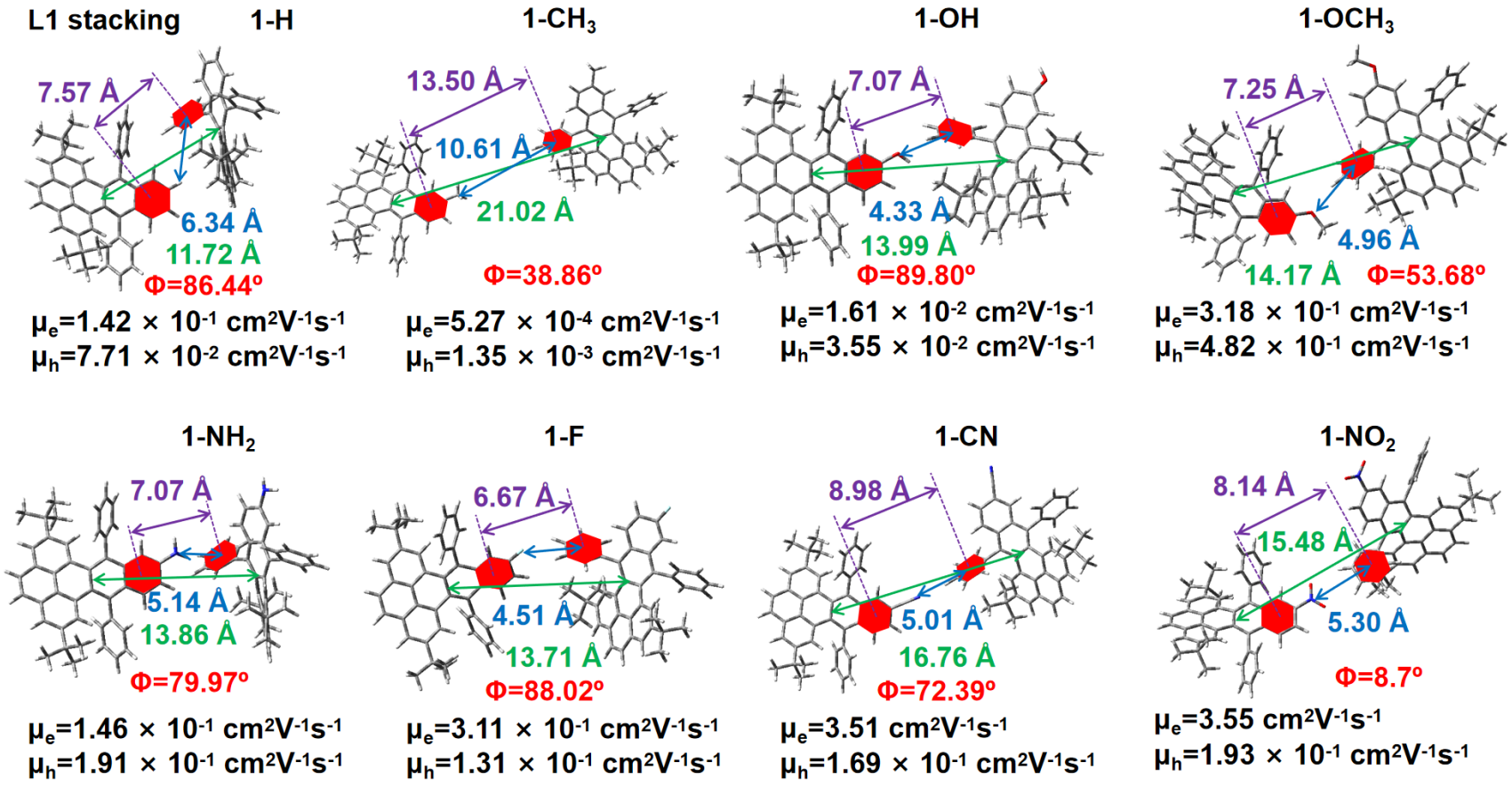


Figure S5. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives in L1 stacking mode, where Φ is the twisted angle of benzene rings.

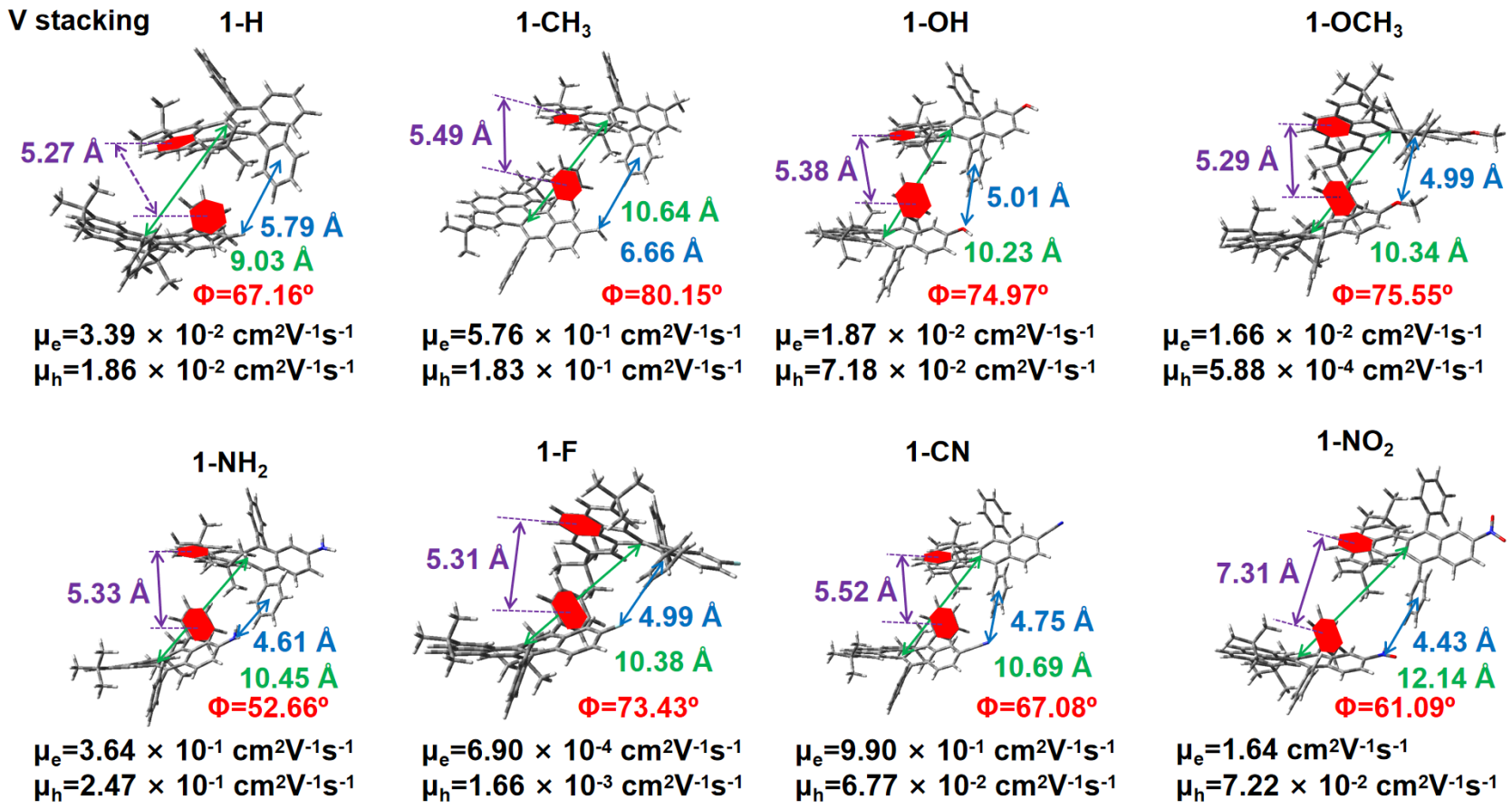


Figure S6. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives in V stacking mode, where Φ is the twisted angle of two benzene rings.

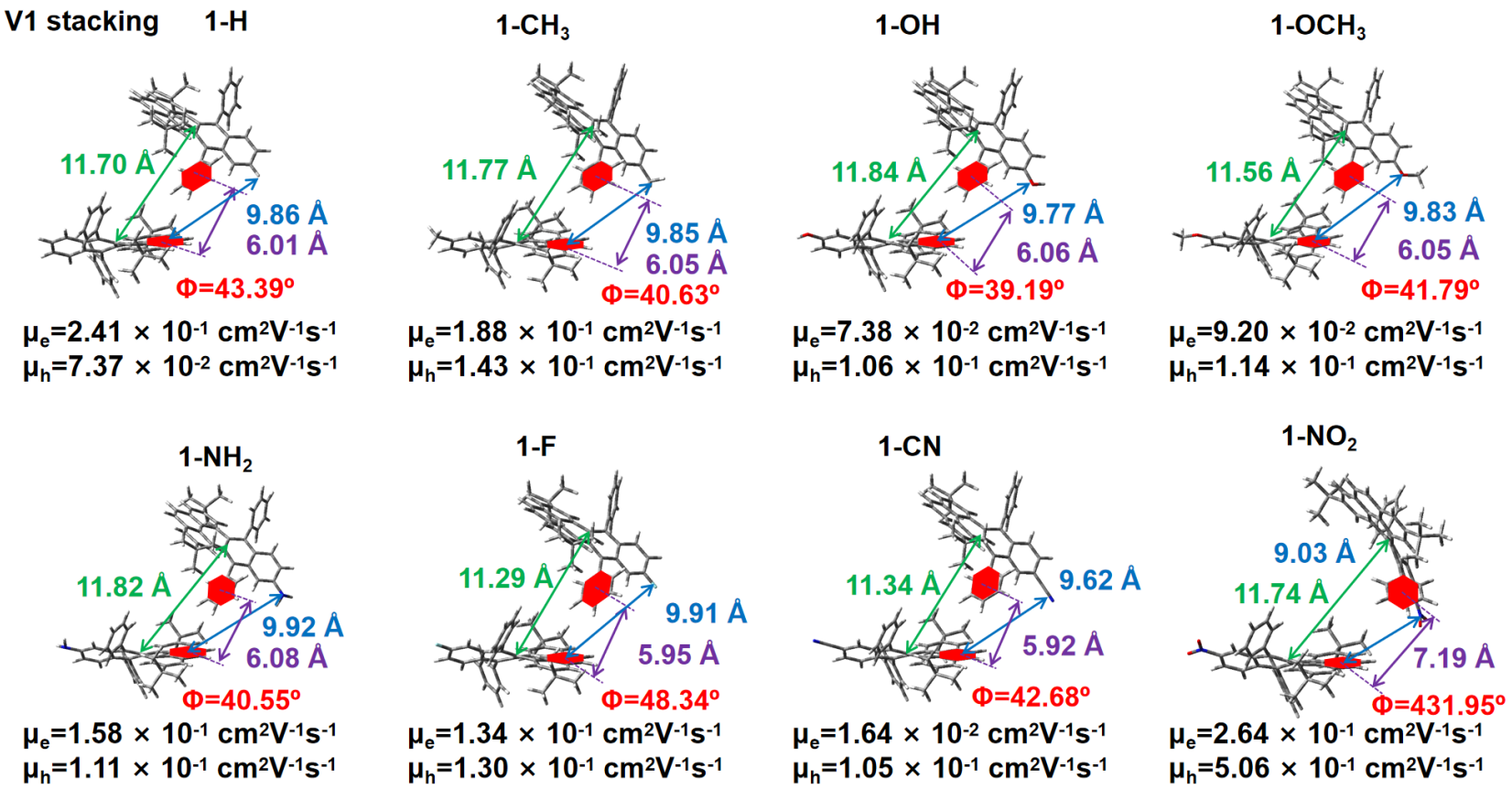


Figure S7. Intermolecular electron and hole mobilities and critical geometrical parameters of 1-H and its derivatives in V1 stacking mode, where Φ is the twisted angle of two benzene rings.

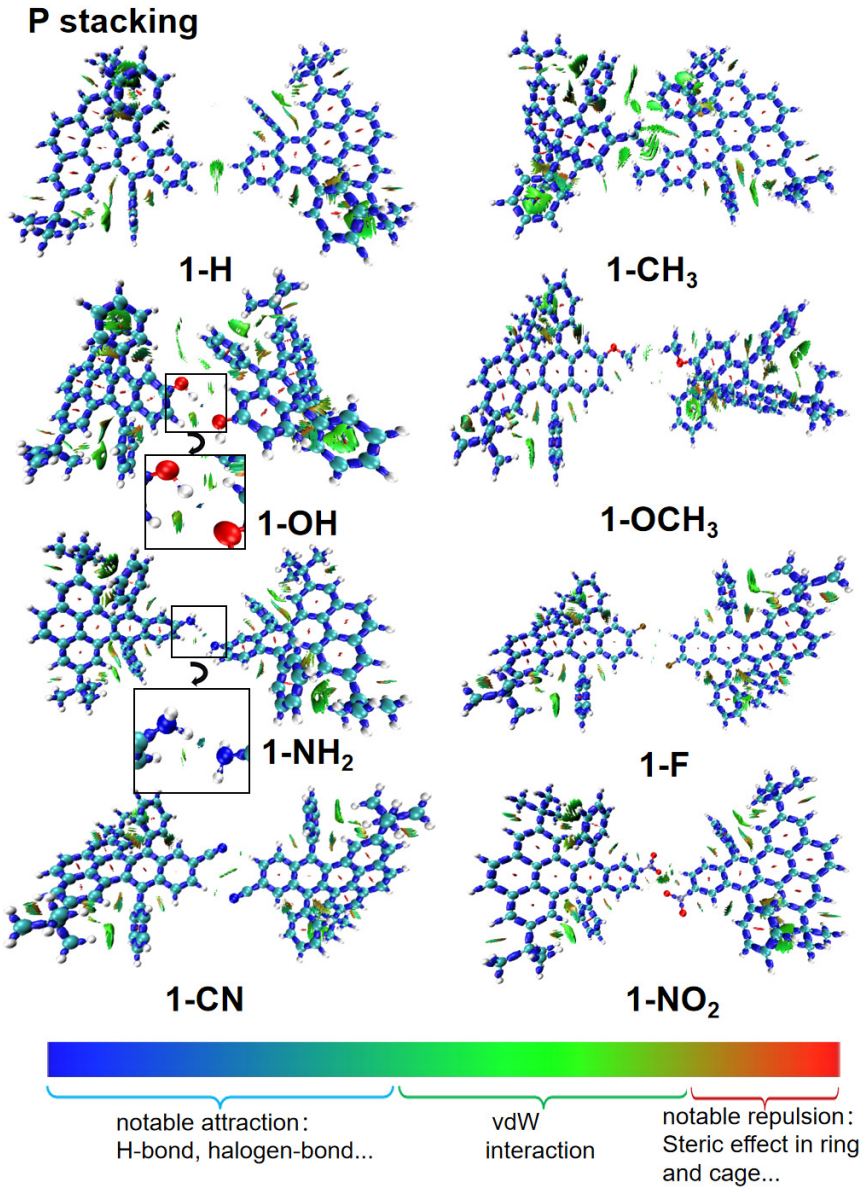


Figure S8. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along P stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

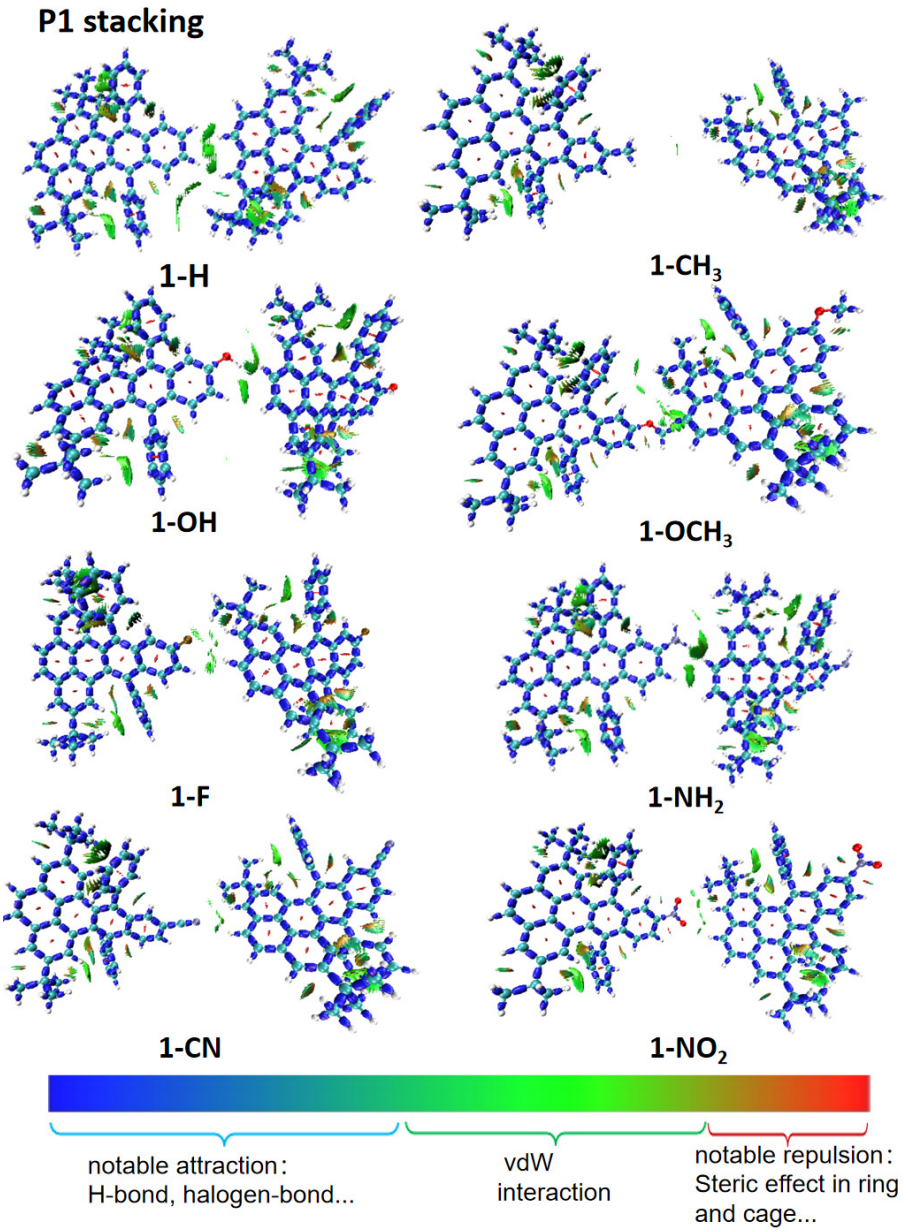


Figure S9. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along P1 stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

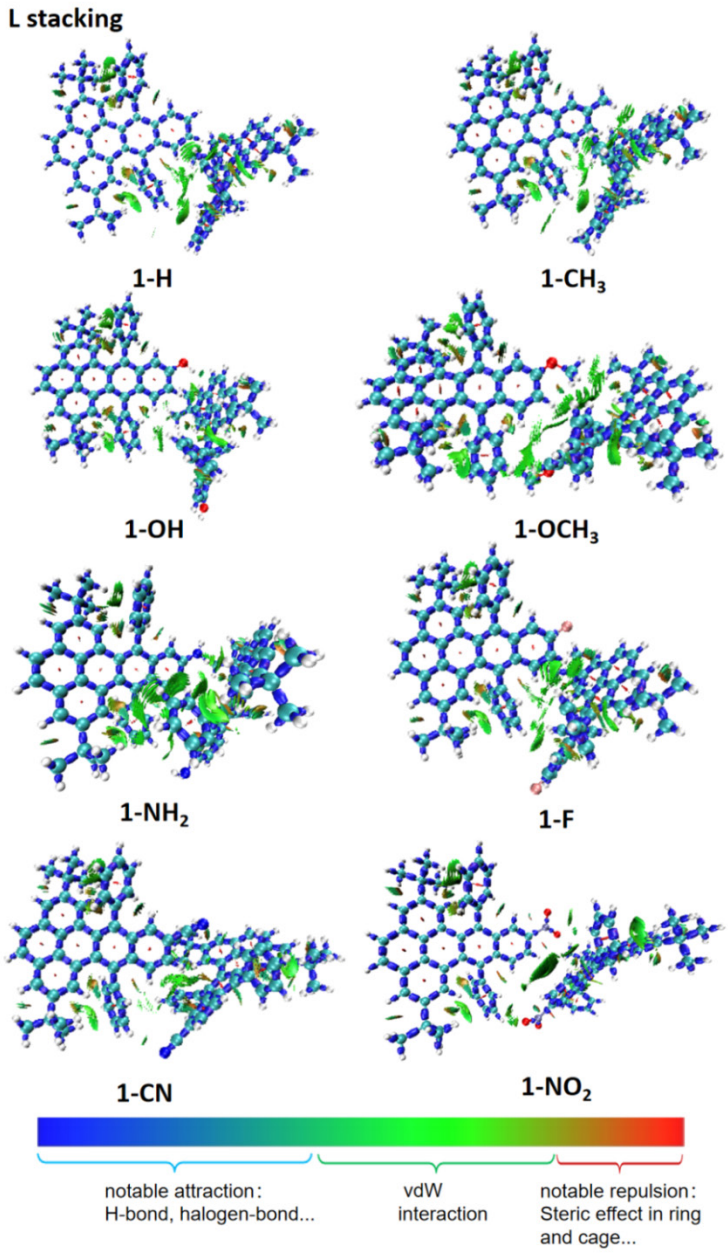


Figure S10. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along L stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

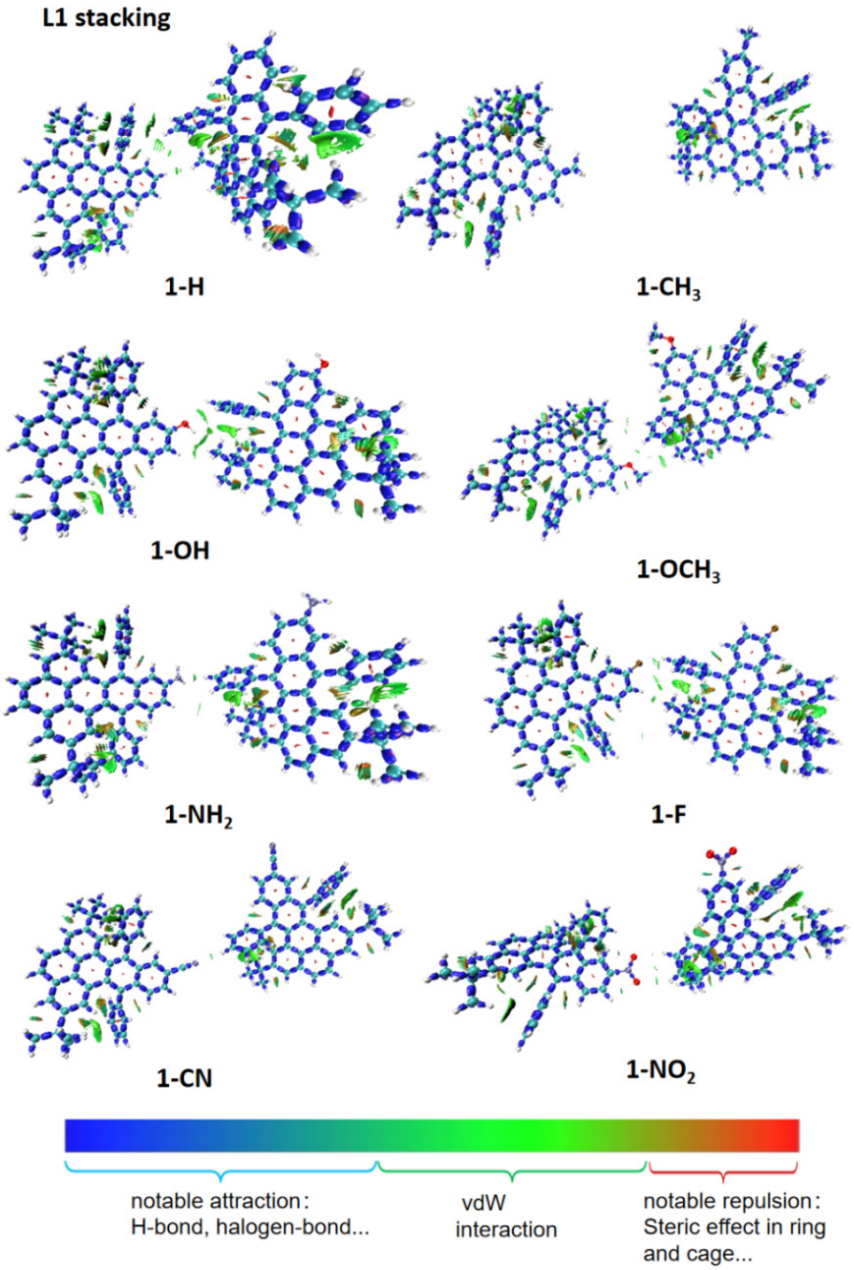


Figure S11. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along L1 stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

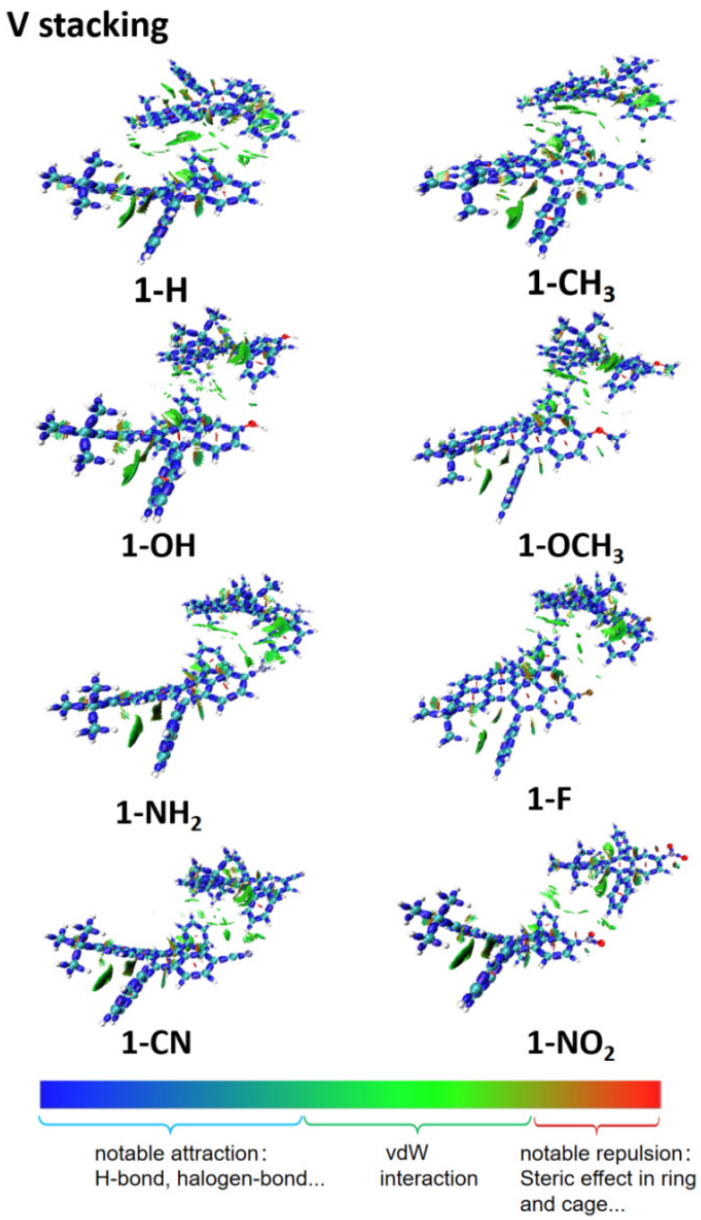


Figure S12. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along V stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

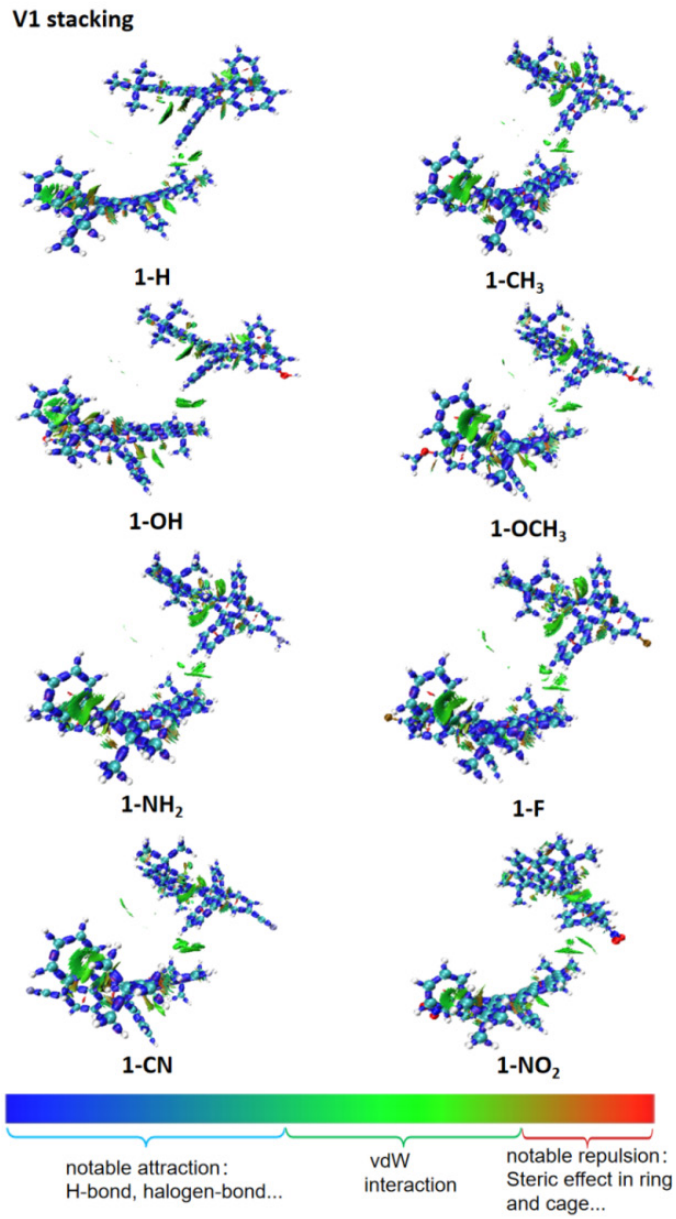


Figure S13. Interaction region indicator (IRI) of chemical bonds and weak interactions for the 1-H and its derivatives dimers along V1 stacking, which were computed by Gaussian 09 at B3LYP-GD2/6-311G**//B3LYP/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

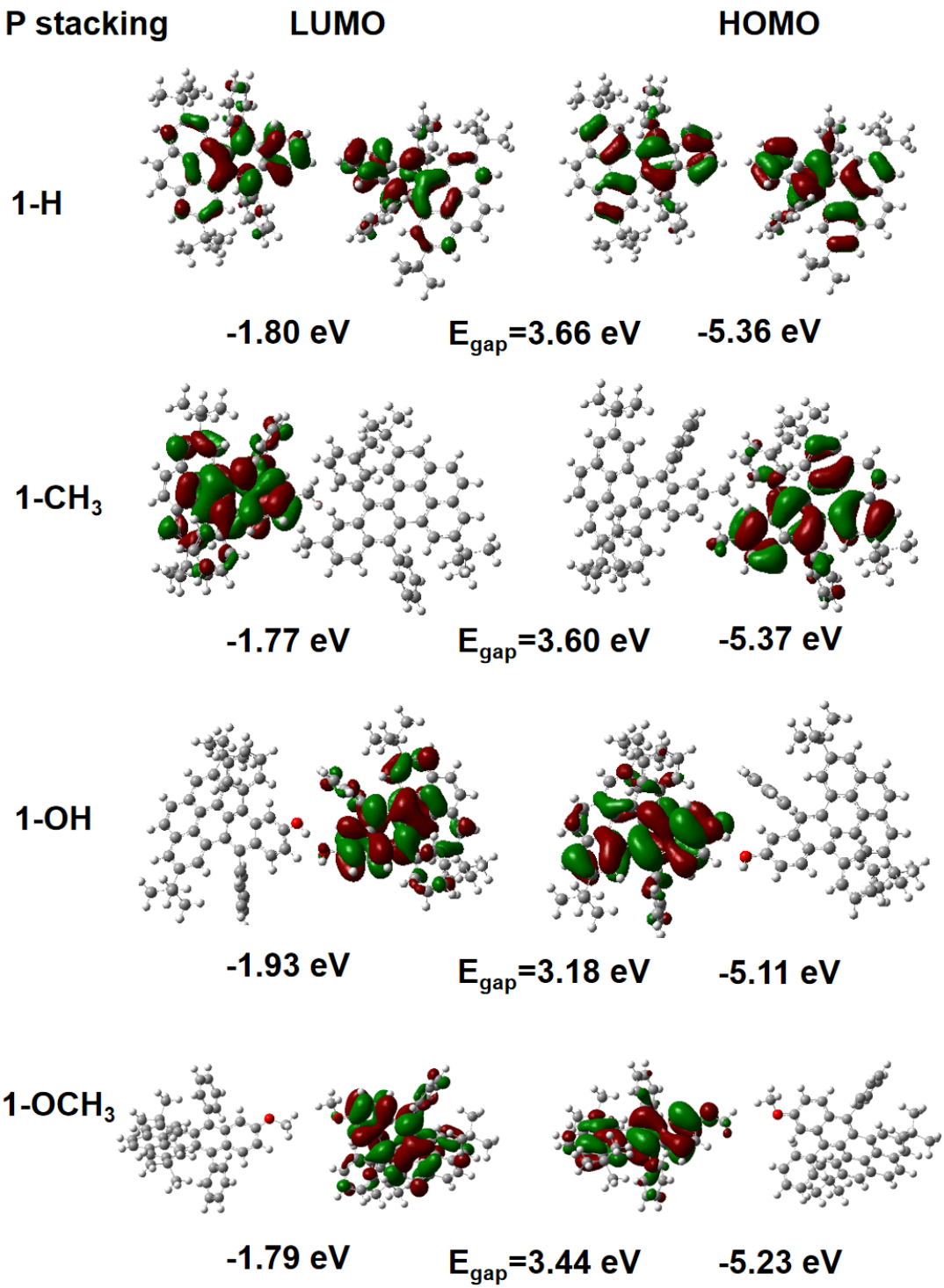


Figure S14. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along P stacking direction.

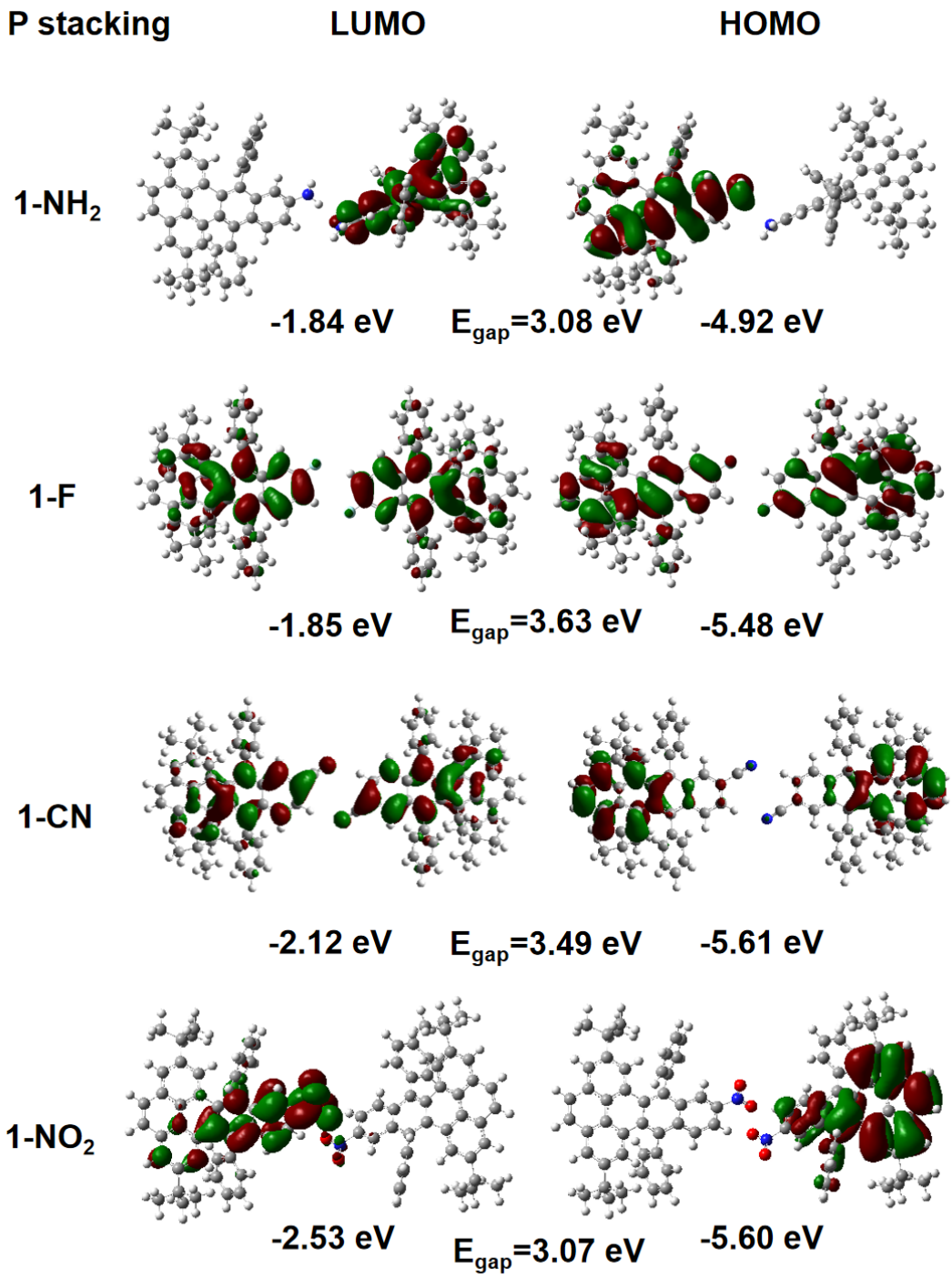


Figure S15. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along P stacking direction.

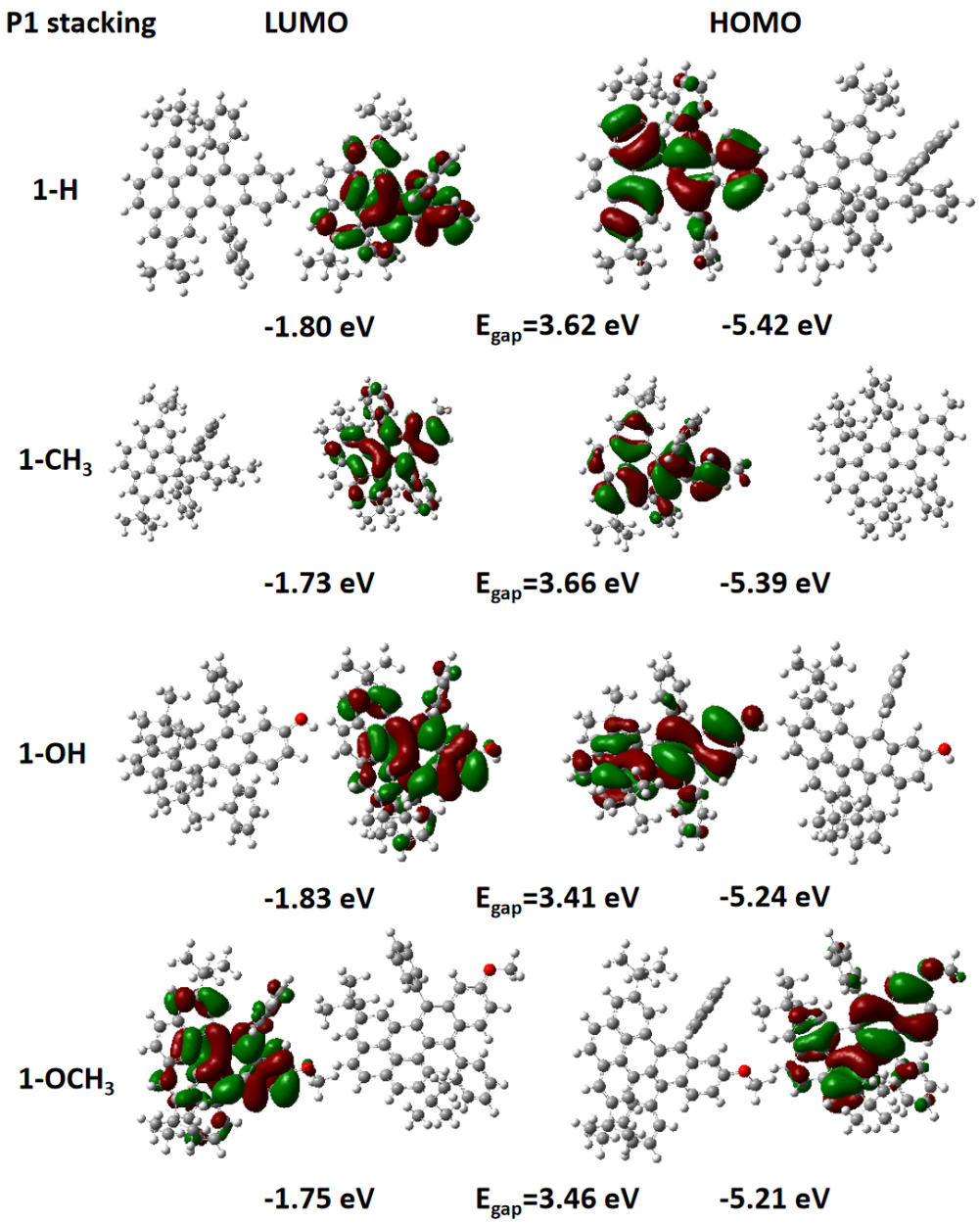


Figure S16. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along P1 stacking direction.

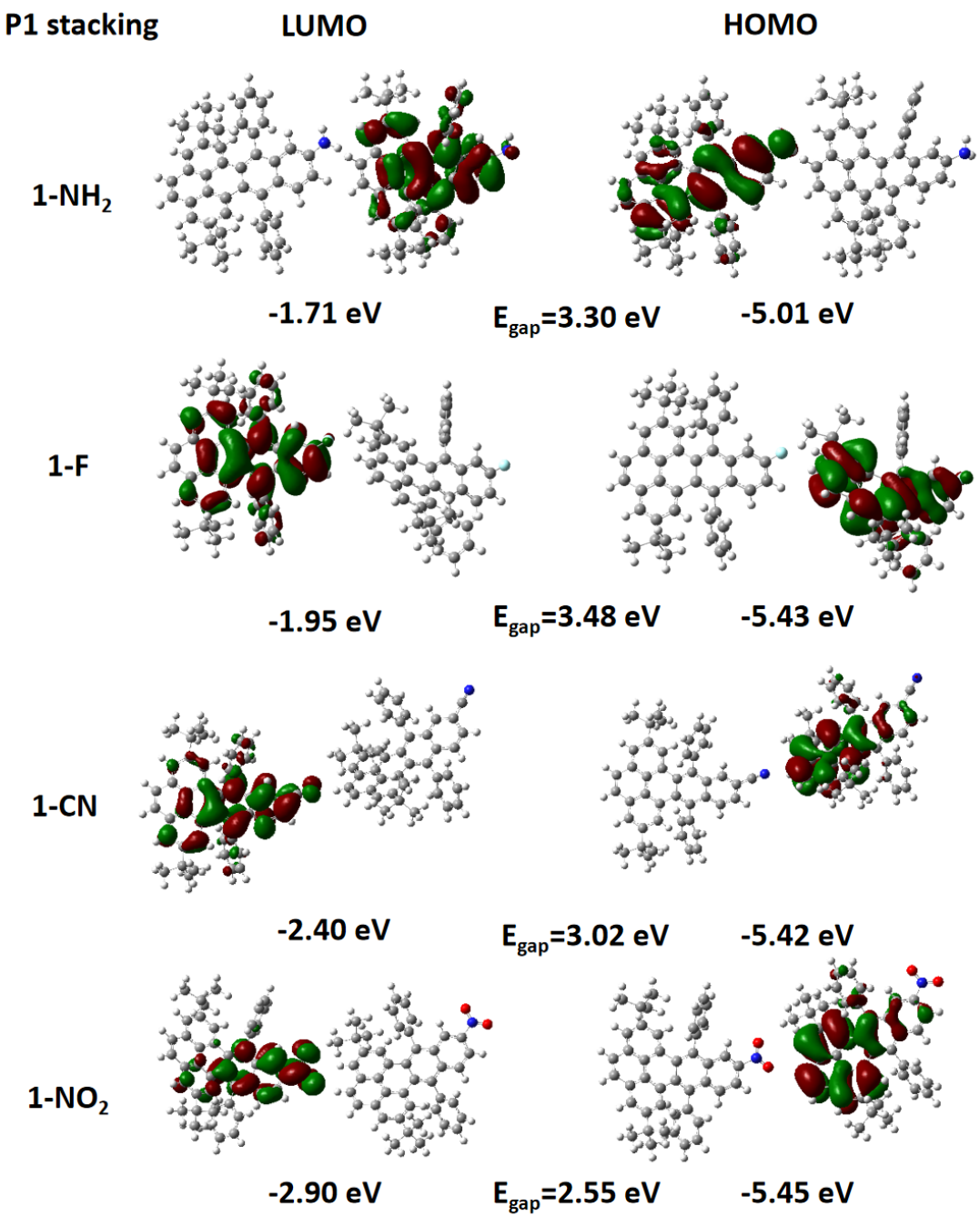


Figure S17. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along P1 stacking direction.

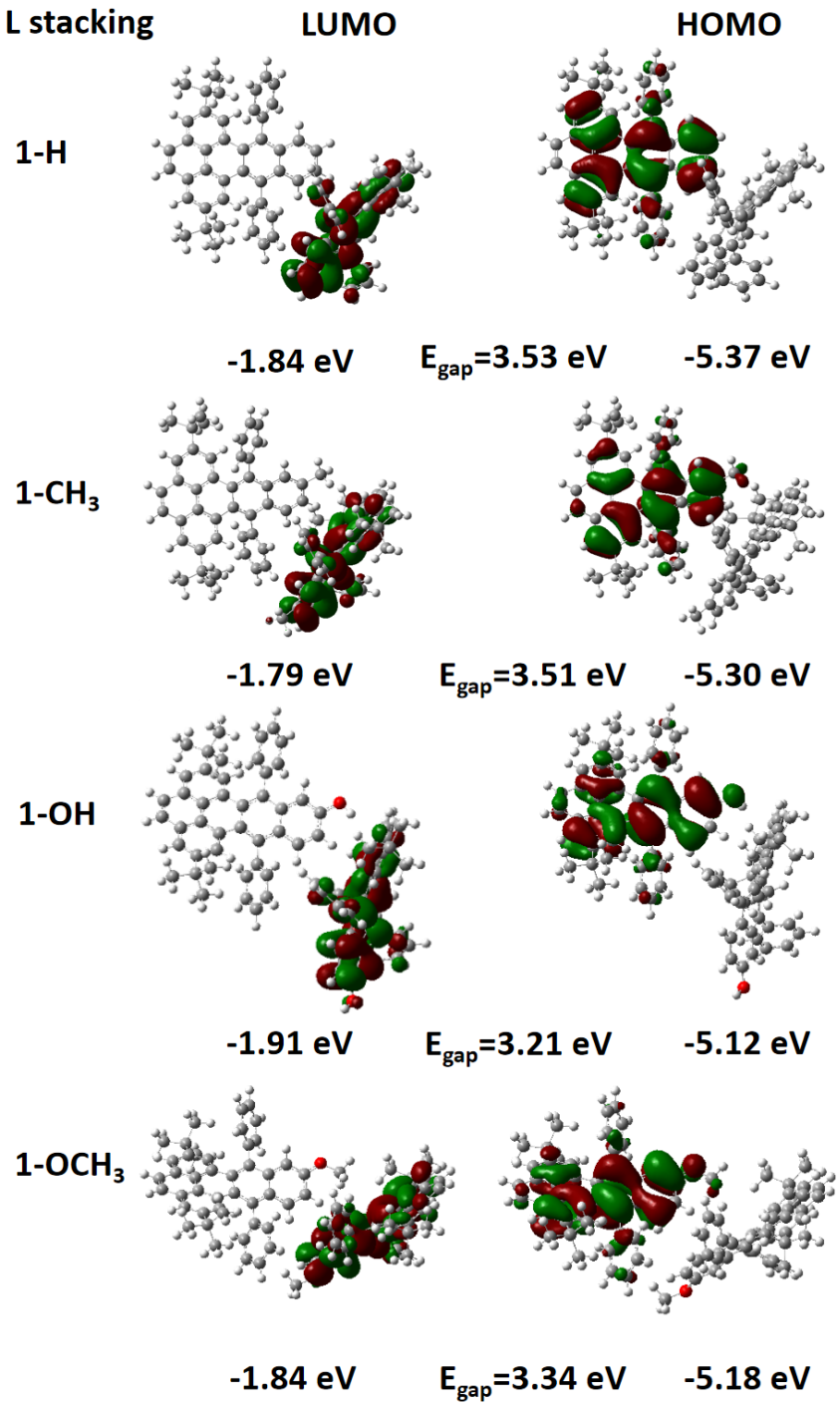


Figure S18. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along L stacking direction.

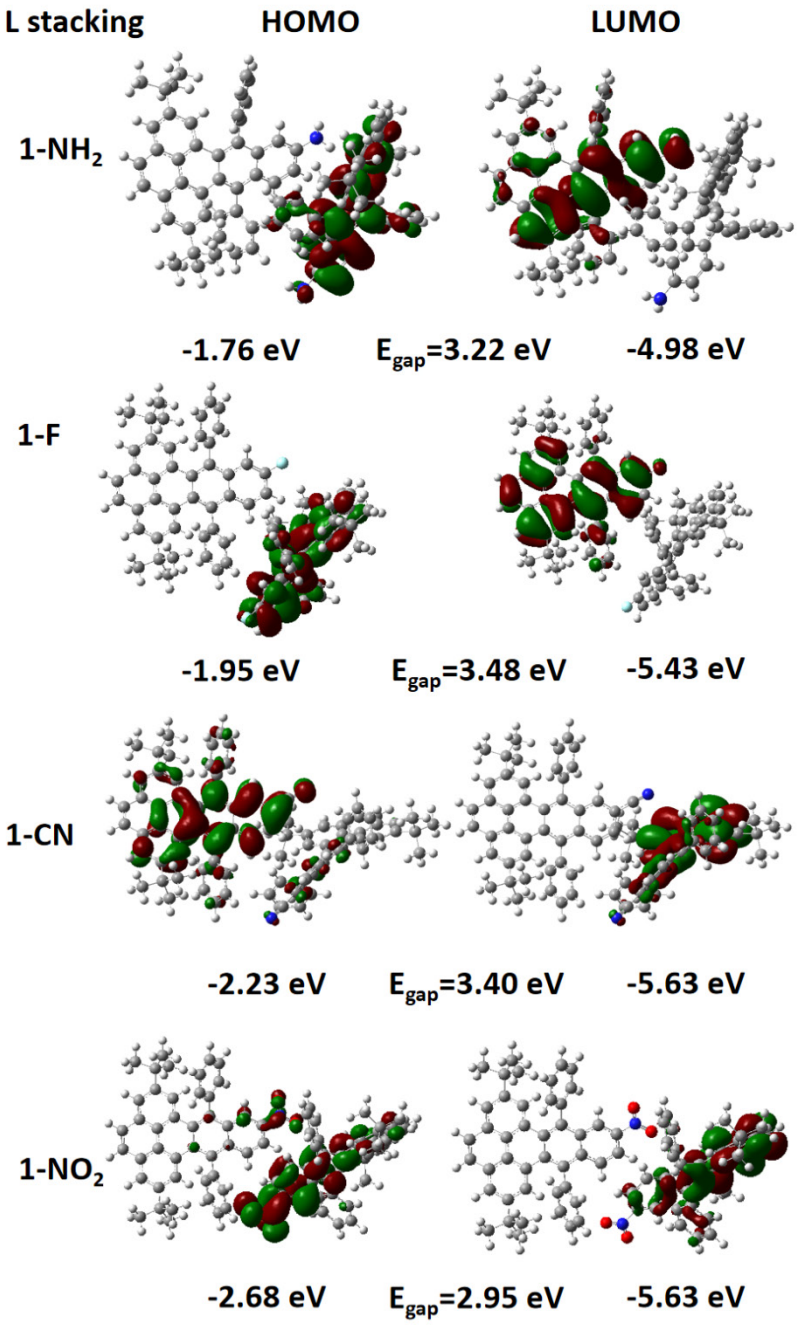


Figure S19. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along L stacking direction.

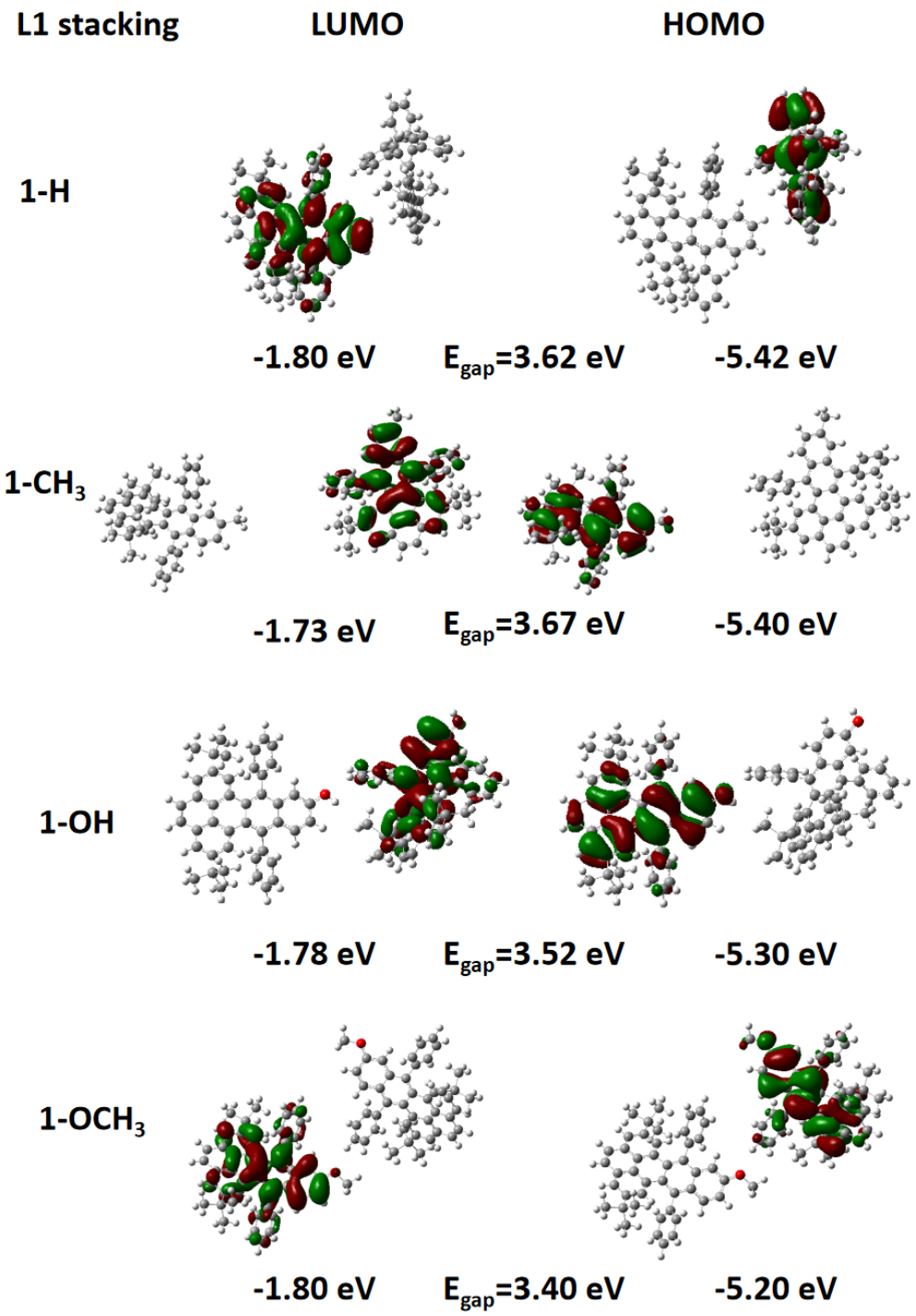


Figure S20. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along L1 stacking direction.

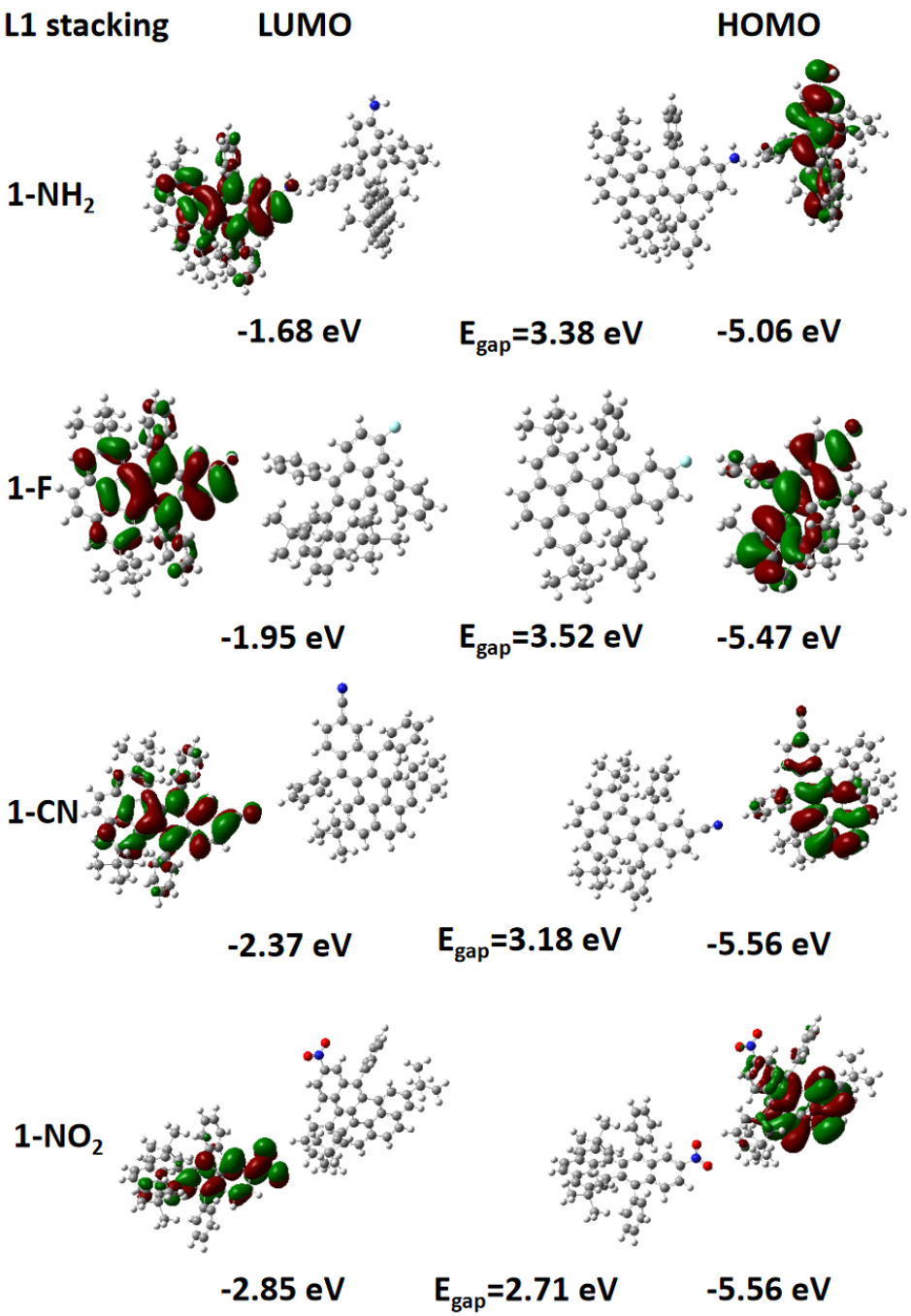


Figure S21. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along L1 stacking direction.

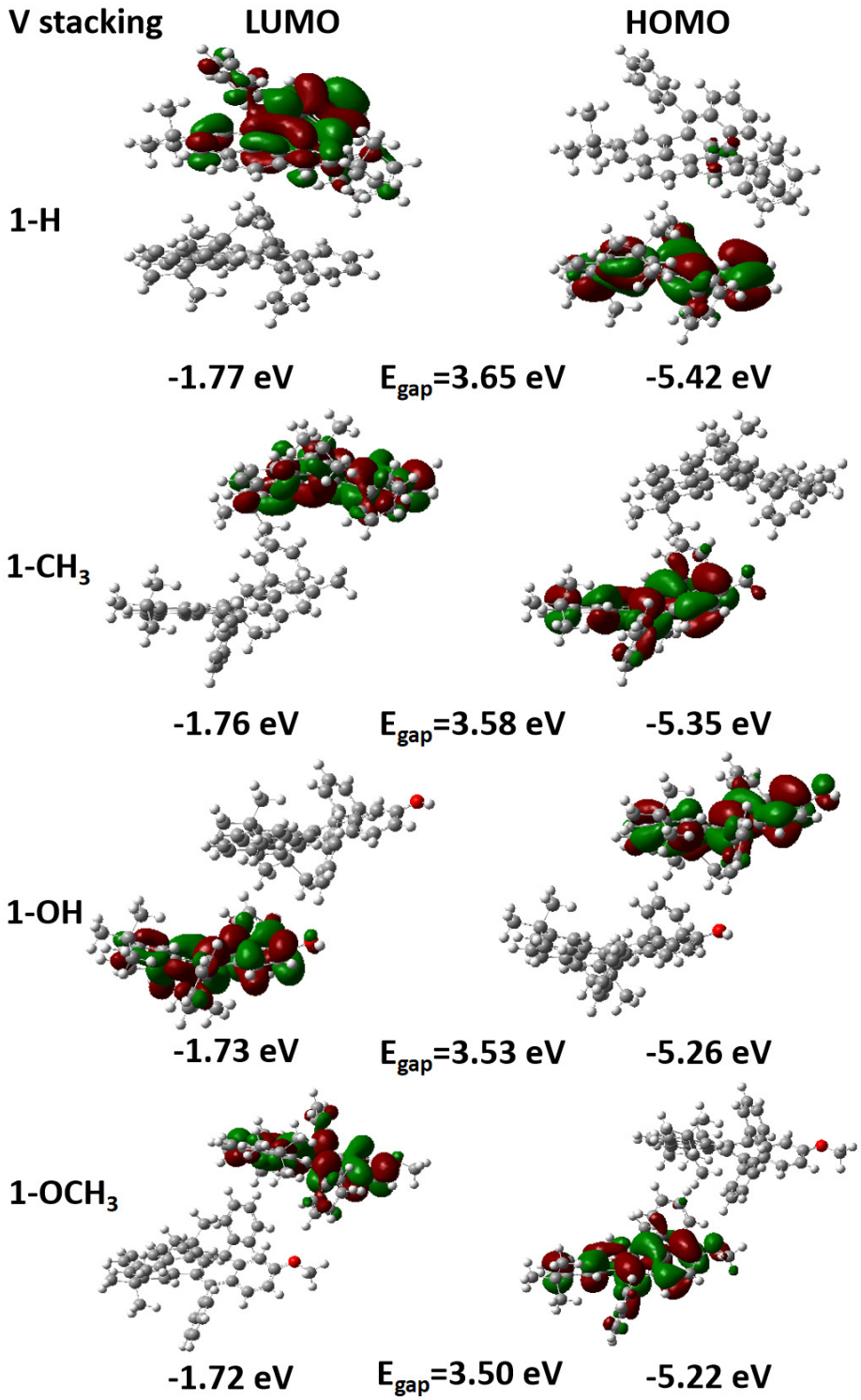


Figure S22. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along V stacking direction.

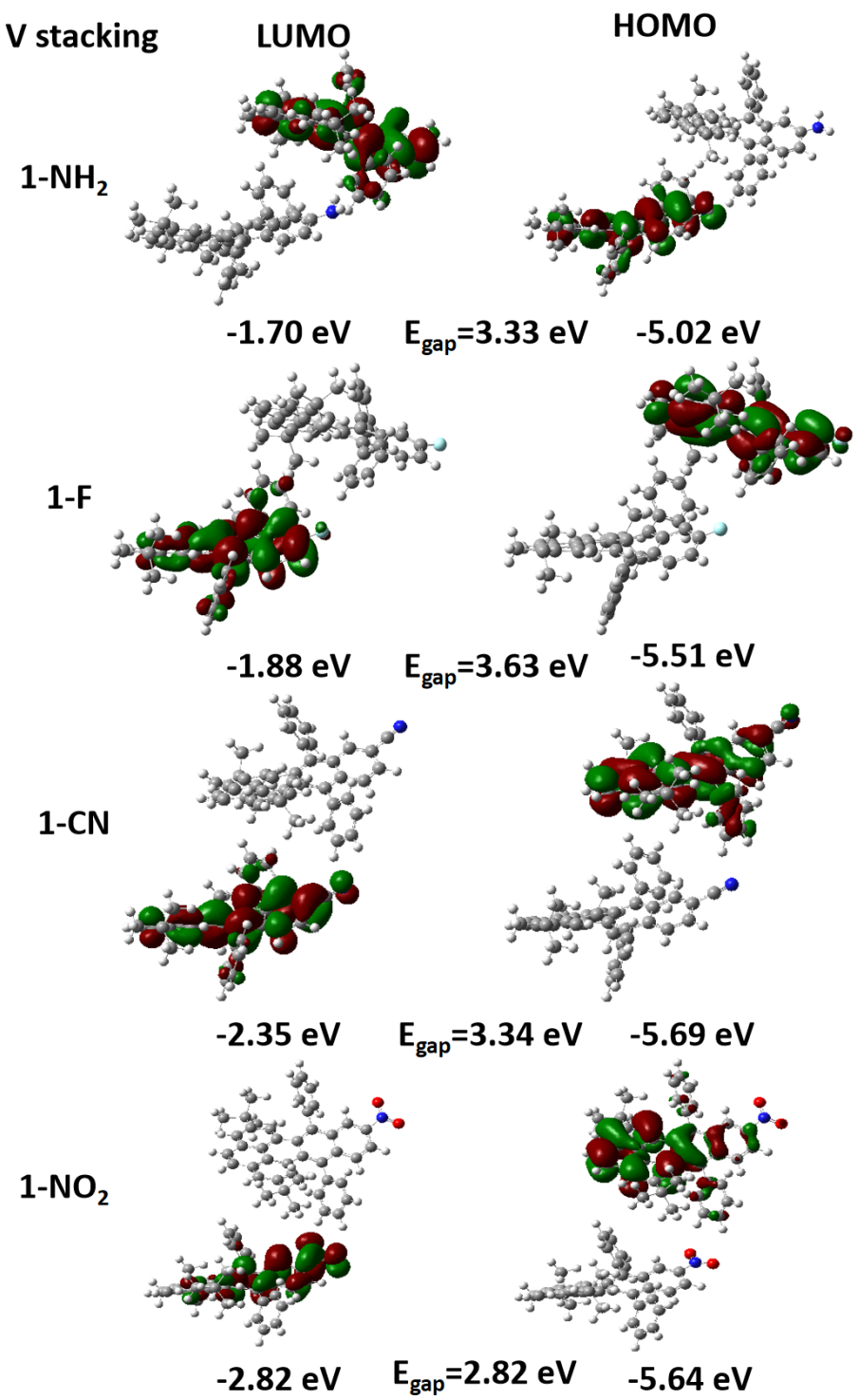


Figure S23. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along V stacking direction.

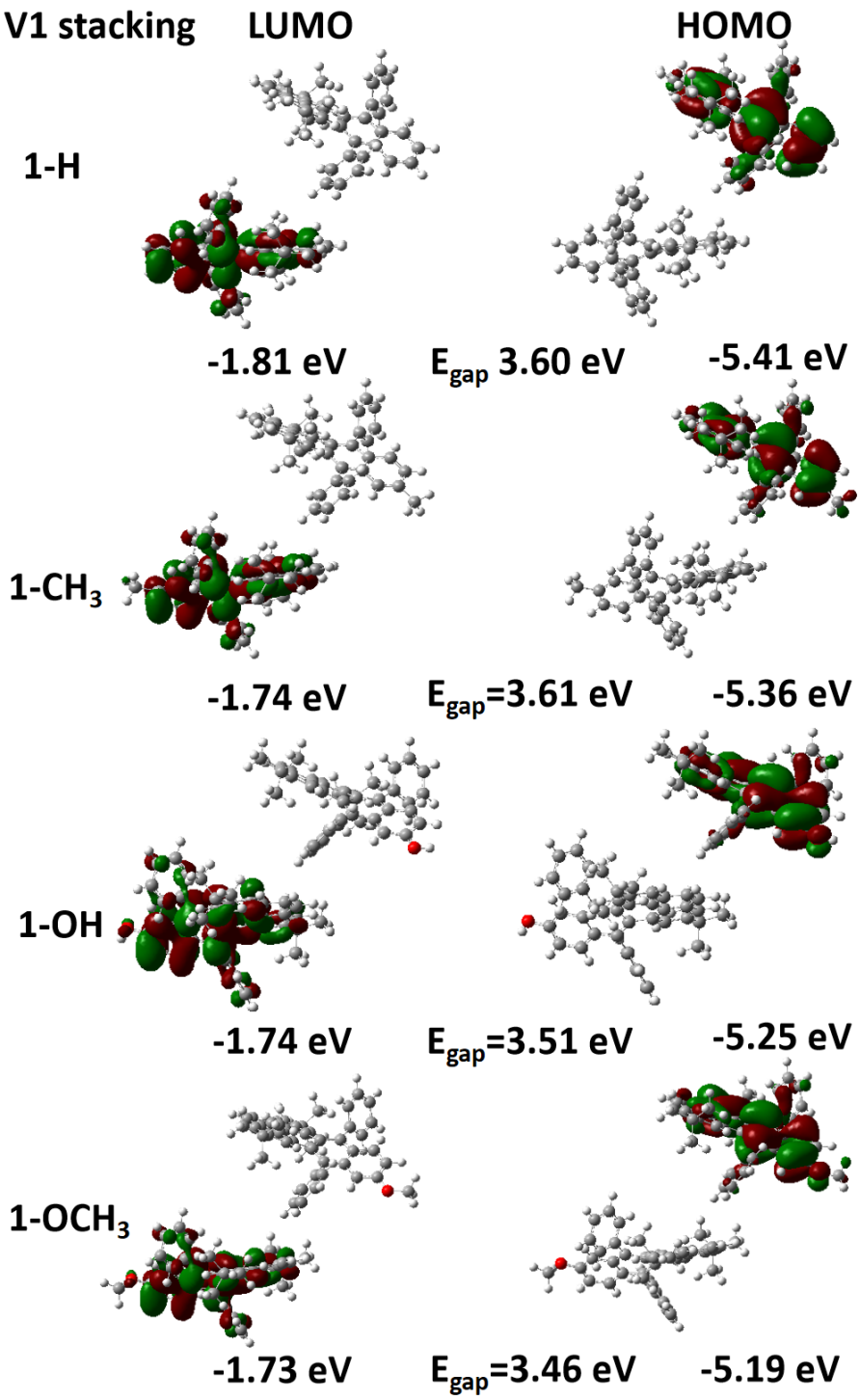


Figure S24. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH and 1-OCH_3 dimers along V1 stacking direction.

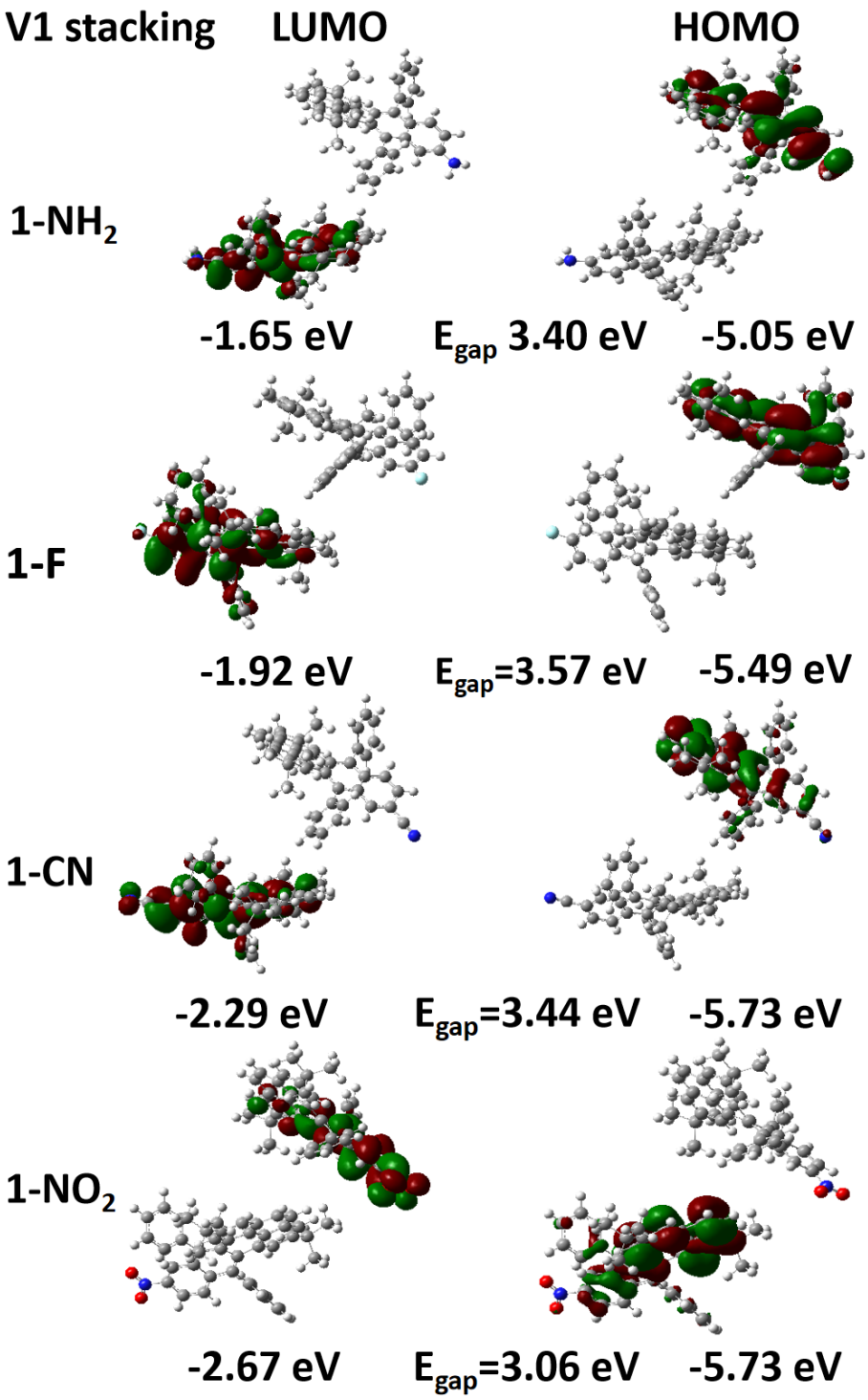


Figure S25. Energy levels of HOMOs and LUMOs at B3LYP/6-311G** level for 1-NH_2, 1-F, 1-CN and 1-NO_2 dimers along V1 stacking direction.

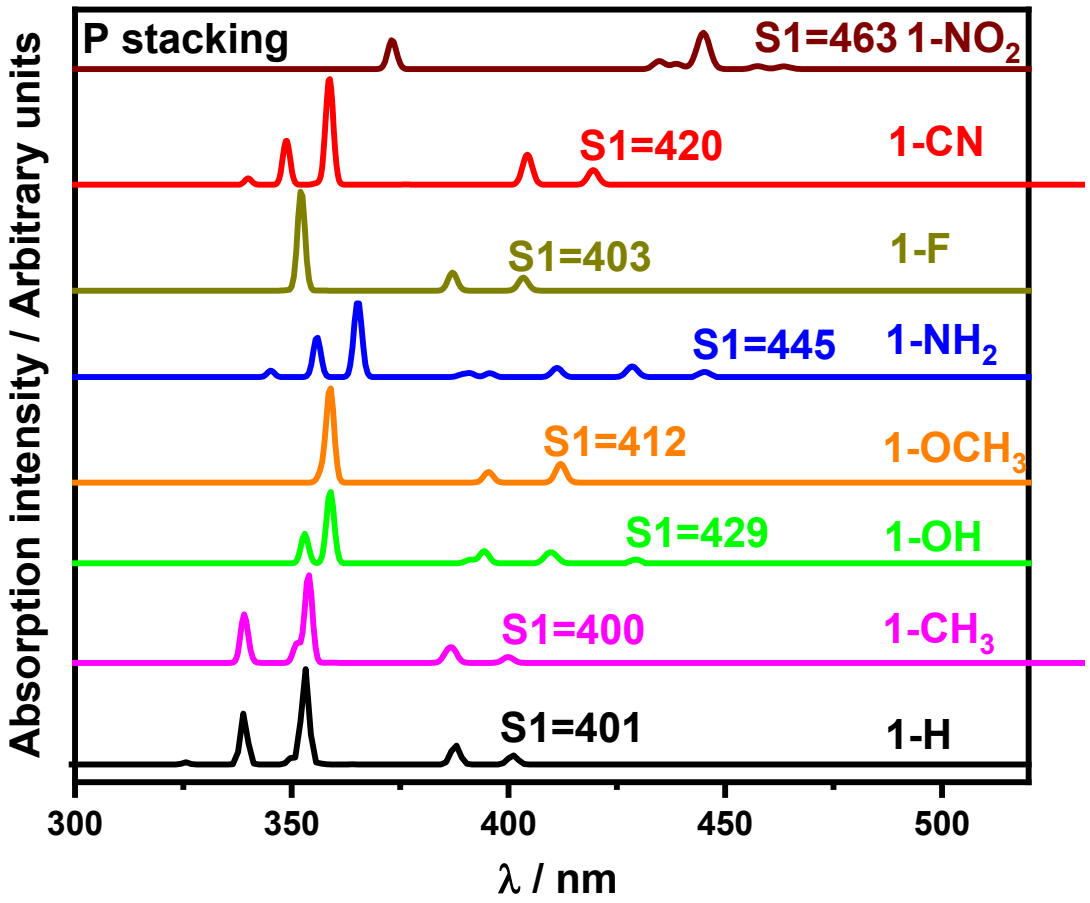


Figure S26. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along P stacking direction.

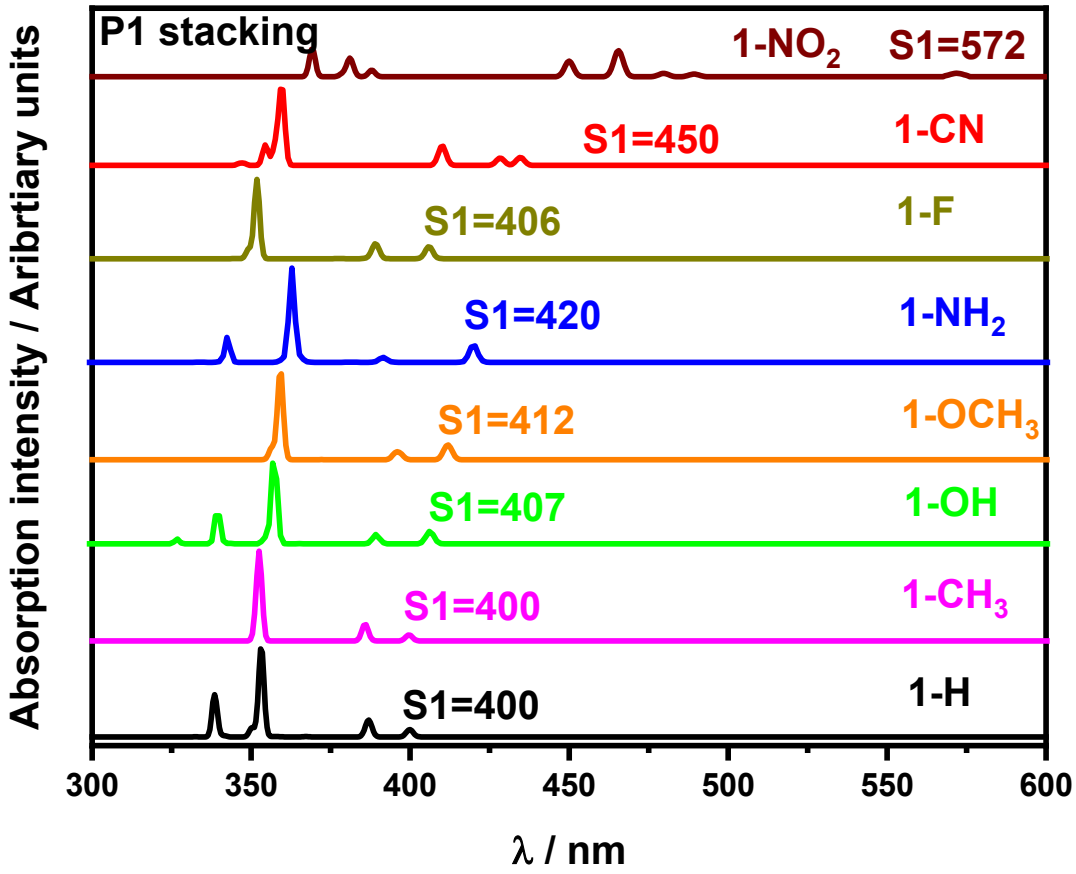


Figure S27. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along P1 stacking direction.

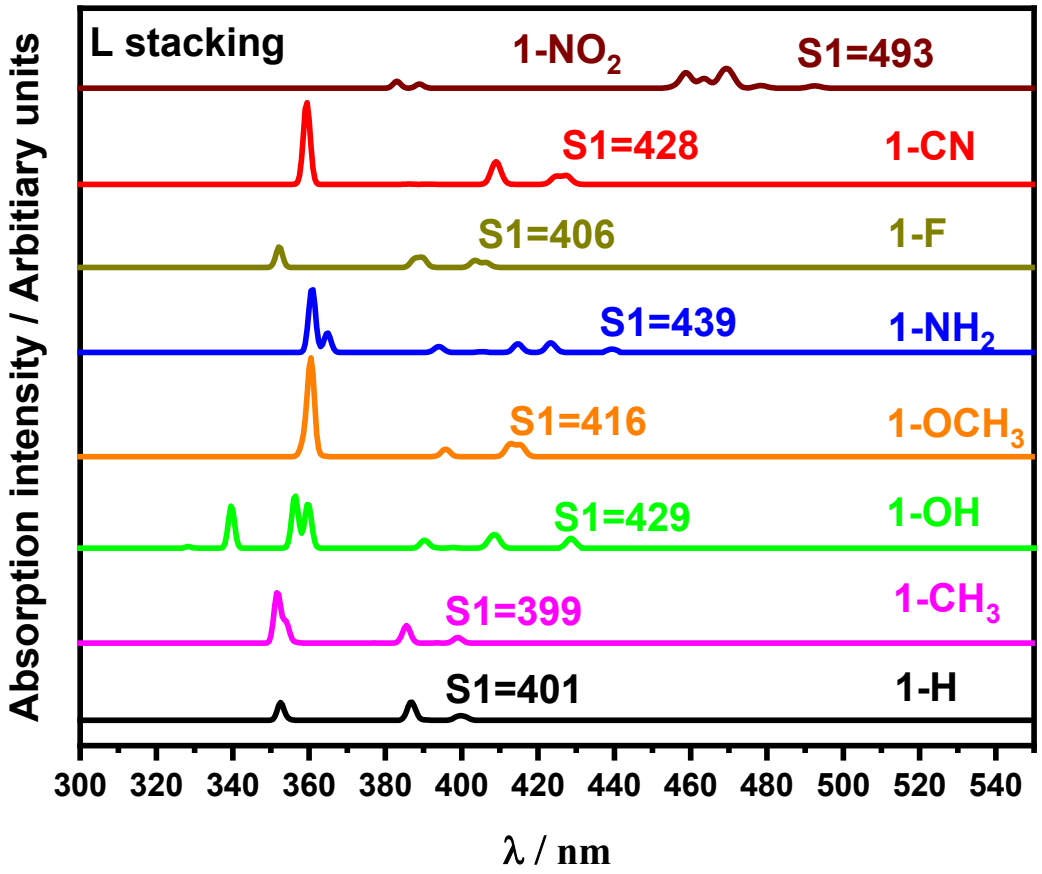


Figure S28. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along L stacking direction.

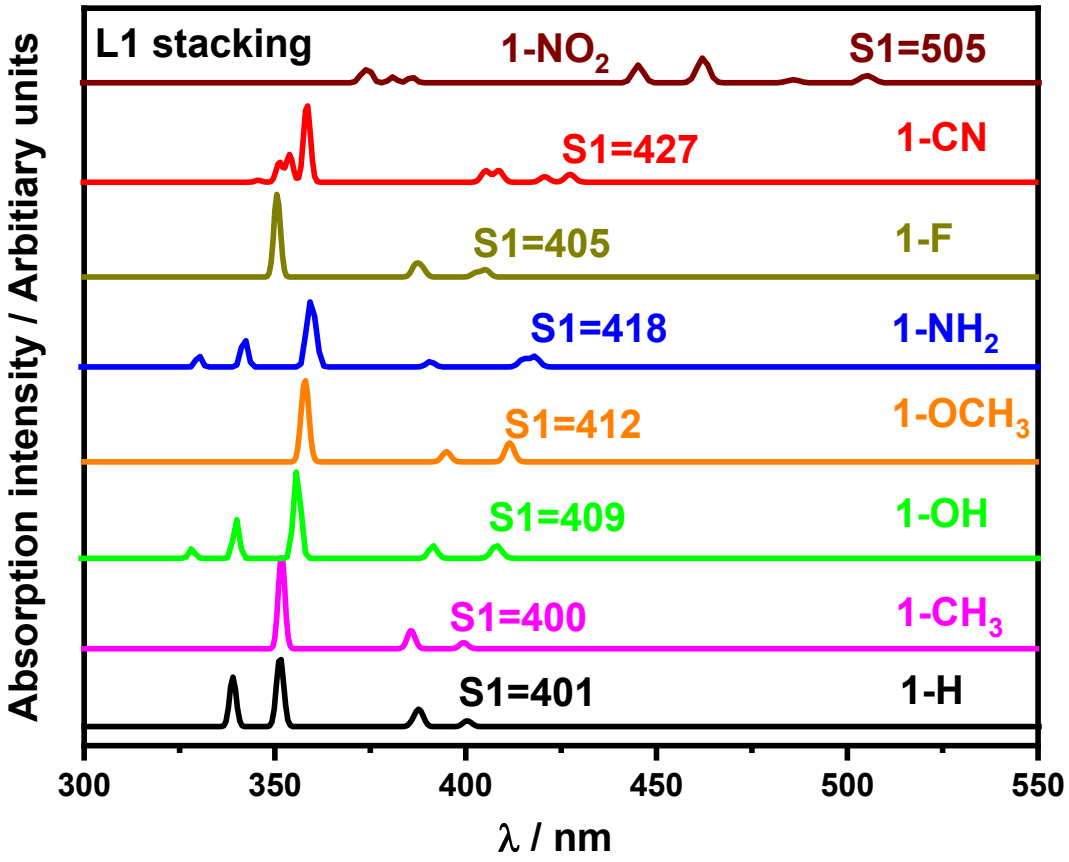


Figure S29. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along L1 stacking direction.

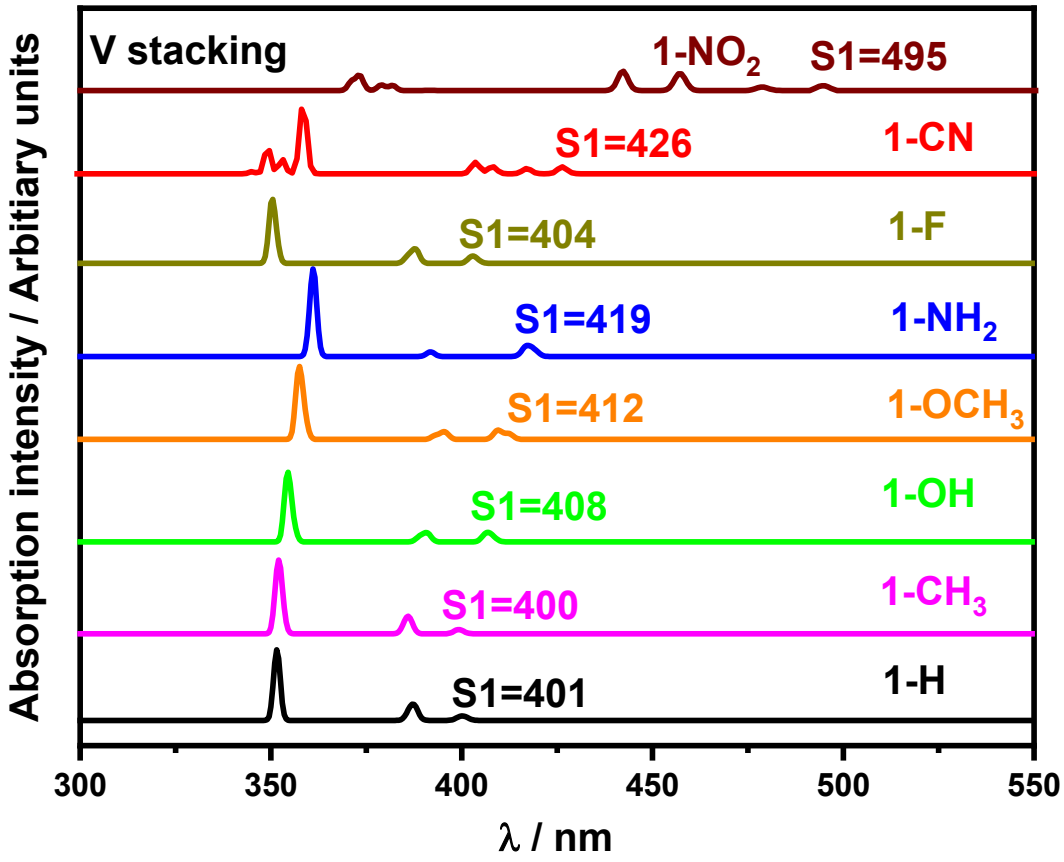


Figure S30. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along V stacking direction.

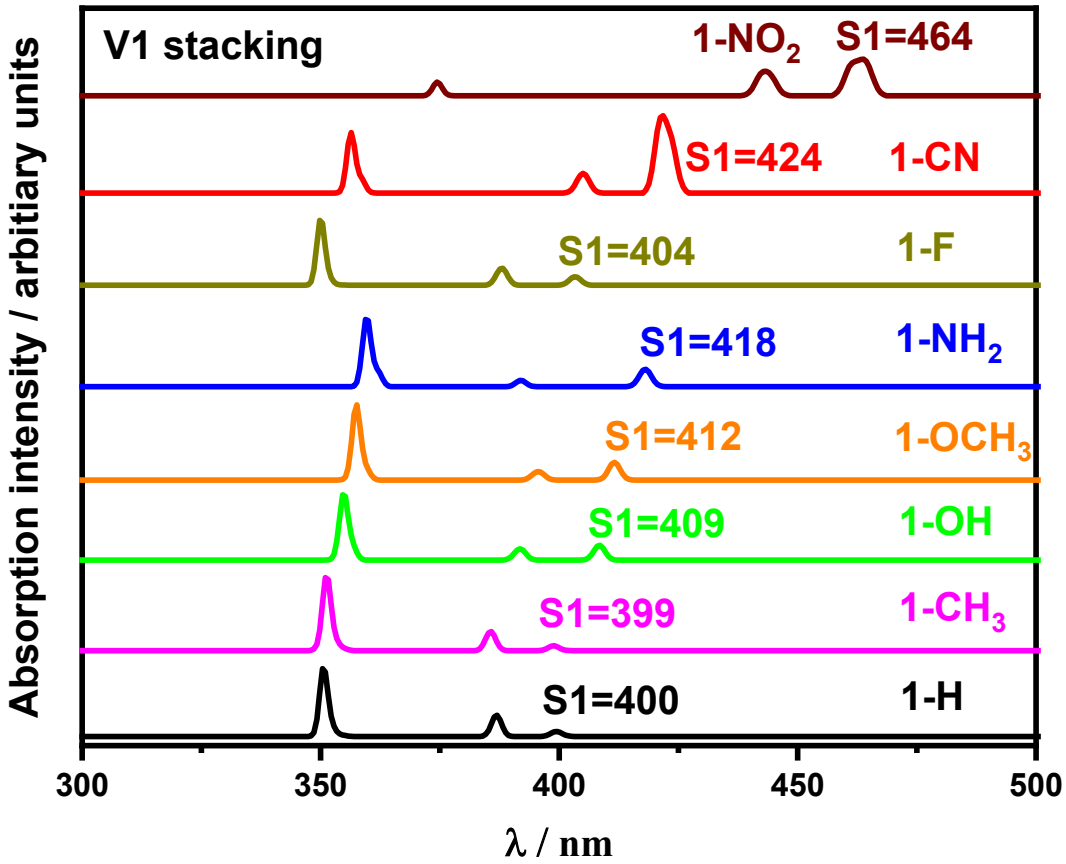


Figure S31. TD-DFT spectra at B3LYP/6-311G** level of dimers for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 along V1 stacking direction.

Table S1. Benchmark calculation to get the proper computational level, taken the UV-vis peaks of 1-CH_3 and its experiment results as standard. The 6-311G** basis set is used for all functionals except that the def2-TZVPP basis set is used for the M06-2X functional.

Species	Functionals	LUMO / eV	HOMO / eV	[a]E_{gap} / eV	S1 / nm	S4 / nm	S13 / nm
1-CH_3	B3LYP	-1.72	-5.40	3.67	399	339	280
	B3LYP[b]	-1.77	-5.46	3.69	398	342	280
	M06-2X	-0.99	-6.58	5.59	343	296	240
	CAM-B3LYP	-0.57	-6.62	6.05	338	294	235
	ωB97XD	-0.01	-7.17	7.16	334	293	233
3a[c]	-	-	-5.32	-	400[d]/425[e]	333[f]/343[g]	265[h]

[a]E_{gap} is the energy difference between HOMO and LUMO.

[b]With the methylene chloride solvent.

[c]From Ref. *Dyes Pigments* **2015**, *112*, 176-182.

[d]Absorption shoulder peak in methylene chloride solvent which was not pointed out by authors.

[e]Absorption shoulder peak in thin film which was not pointed out by authors.

[f]Absorption peak in methylene chloride solvent.

[g]Absorption peak in thin film.

[h]Absorption peak in methylene chloride solvent which was not pointed out by authors.

Table S2. The twisted angles (θ) between the pyrene moieties and naphthalene units of 1-H and its derivatives.

Species	Twisted angle / º	Species[a]	Twisted angle[a] / º
1-H	32.87		
1-CH_3	32.68	3a	28.56
1-OH	32.57		
1-OCH_3	32.61	3b	29.74
1-NH_2	32.58		
1-F	32.50	3c	36.26
1-CN	33.02		
1-NO_2	32.95		

[a] From Ref. *Dyes Pigments* **2015**, *112*, 176-182.

Table S3. Computational energies at B3LYP/6-311G** level for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2 and the corresponding binding energies for the dimers along six different stacking patterns.

Species	Stacking patterns	Electronic energy (EE) / Hartree	Binding energy[a] / kcal/mol
1-H monomer	-	-1700.034584	
1-H dimers	P	-3400.527213	-1.62
	P1	-3400.530977	-3.98
	L	-3400.542901	-11.47
	L1	-3400.530091	-3.43
	V	-3400.539011	-9.03
	V1	-3400.530983	-3.99
1-CH_3 monomer	-	-1739.362765	
1-CH_3 dimers	P	-3479.203182	-6.83
	P1	-3479.192477	-0.11
	L	-3479.213127	-13.07
	L1	-3479.192373	-0.05
	V	-3479.202457	-6.38
	V1	-3479.198512	-3.90
1-OH monomer	-	-1775.277716	
1-OH dimers	P	-3551.033539	-11.48
	P1	-3551.023054	-4.90
	L	-3551.033412	-11.40
	L1	-3551.024371	-5.73
	V	-3551.027941	-7.97
	V1	-3551.021420	-3.87
1-OCH_3 monomer	-	-1814.587124	
1-OCH_3 dimers	P	-3629.645443	-1.13
	P1	-3629.654287	-6.67
	L	-3629.660055	-10.29
	L1	-3629.650144	-4.08
	V	-3629.658490	-9.31
	V1	-3629.650033	-4.01

1-NH_2 monomer	-	-1755.408791	
1-NH_2 dimers	P	-3511.293141	-7.32
	P1	-3511.290903	-5.92
	L	-3511.307940	-16.61
	L1	-3511.286471	-3.14
	V	-3511.296992	-9.74
	V1	-3511.287594	-3.84
1-F monomer	-	-1799.299373	
1-F dimers	P	-3599.061681	-4.25
	P1	-3599.062668	-4.87
	L	-3599.071638	-10.50
	L1	-3599.061644	-4.23
	V	-3599.068529	-8.55
	V1	-3599.061769	-4.31
1-CN monomer	-	-1792.300579	
1-CN dimers	P	-3585.077264	-6.88
	P1	-3585.072985	-4.19
	L	-3585.083345	-10.70
	L1	-3585.071454	-3.23
	V	-3585.080075	-8.64
	V1	-3585.073206	-4.33
1-NO_2 monomer	-	-1904.592597	
1-NO_2 dimers	P	-3809.662605	-5.76
	P1	-3809.663790	-6.50
	L	-3809.674086	-12.96
	L1	-3809.662724	-5.83
	V	-3809.664594	-7.00
	V1	-3809.657548	-2.58

[a]The binding energies are calculated as the difference between the total energy of the dimer and twice the total energy of a single molecule.

Table S4. The twisted angles between the pyrene moieties and naphthalene units (θ) of each molecule of the dimers for 1-H and its derivatives.

Species	Stacking patterns	[a]Twisted angle / º
1-H	P	32.82/32.82
1-CH_3		32.99/32.80
1-OH		32.68/32.79
1-OCH_3		32.55/32.63
1-NH_2		32.81/32.78
1-F		32.54/32.54
1-CN		33.16/33.17
1-NO_2		33.06/32.87
1-H	P1	32.83/32.89
1-CH_3		32.78/32.82
1-OH		32.16/32.29
1-OCH_3		32.74/32.66
1-NH_2		32.16/32.29
1-F		32.51/32.49
1-CN		33.18/33.12
1-NO_2		33.00/32.89
1-H	L	32.93/32.81
1-CH_3		32.80/32.55
1-OH		32.51/32.71
1-OCH_3		32.80/32.41
1-NH_2		32.70/31.91
1-F		32.51/32.63
1-CN		32.47/31.91
1-NO_2		32.90/30.95
1-H	L1	32.84/32.89
1-CH_3		32.70/32.71
1-OH		32.58/32.35
1-OCH_3		32.77/32.54
1-NH_2		32.33/32.56

1-F		32.49/32.36
1-CN		33.05/32.89
1-NO_2		32.90/32.78
1-H		32.73/33.25
1-CH_3		32.49/33.03
1-OH		32.17/32.15
1-OCH_3	V	32.49/32.57
1-NH_2		32.53/32.86
1-F		32.21/32.37
1-CN		33.10/32.88
1-NO_2		32.88/31.95
1-H		32.86/32.79
1-CH_3		32.74/32.65
1-OH		32.61/32.54
1-OCH_3	V1	32.64/32.59
1-NH_2		32.63/32.51
1-F		32.49/32.48
1-CN		33.02/32.90
1-NO_2		33.13/32.43

[a] Corresponding the twisted angle of each molecule of the dimer, respectively.

Table S5. TD-DFT results at B3LYP/6-311G** level for the three lowest-lying singlet states for 1-H, 1-CH_3, 1-OH, 1-OCH_3, 1-NH_2, 1-F, 1-CN and 1-NO_2.

Species	States	Excitation energy / eV	Oscillator strengths	Wavelength / nm	[a]Dominant orbital transitions contributions (DOTC)
1-H	S1	3.10	0.0258	400.20	H-1→L (75.32%), H→L+1 (22.75%)
	S2	3.20	0.0810	387.08	H→L (93.60%)
	S3	3.53	0.3345	351.19	H→L+1 (70.80%), H-1→L (22.89%)
1-CH_3	S1	3.10	0.0245	399.45	H-1→L (51.82%), H→L (21.27%), H→L+1 (20.02%)
	S2	3.21	0.0727	385.63	H→L (69.55%), H-1→L (22.71%)
	S3	3.52	0.3741	351.75	H→L+1 (60.99%), H-1→L (23.19%)
1-OH	S1	3.03	0.0603	408.82	H→L (72.18%)
	S2	3.17	0.0476	391.57	H-1→L (63.63%), H→L (20.44%)
	S3	3.49	0.3371	355.38	H→L+1 (63.83%), H-2→L (34.53%)
1-OCH_3	S1	3.01	0.0722	411.93	H→L (75.91%)
	S2	3.14	0.0348	395.38	H-1→L (61.86%)
	S3	3.46	0.3654	358.05	H→L+1 (64.82%), H-1→L (25.59%)
1-NH_2	S1	2.96	0.0728	418.52	H→L (84.71%)
	S2	3.17	0.0197	391.64	H-1→L (56.09%), H→L+1 (31.28%)
	S3	3.44	0.3576	360.44	H→L+1 (54.23%), H-1→L (37.39%)
1-F	S1	3.07	0.0421	404.11	H→L (67.31%)
	S2	3.20	0.0741	388.04	H-1→L (73.15%)
	S3	3.54	0.3115	350.53	H→L+1 (40.61%), H-2→L (33.68%)
1-CN	S1	2.93	0.0491	422.54	H→L (82.33%)
	S2	3.06	0.0861	404.75	H-1→L (89.22%)
	S3	3.47	0.3108	357.21	H-1→L+1 (75.98%)
1-NO_2	S1	2.69	0.0256	461.12	H→L (76.94%)
	S2	2.82	0.1444	440.35	H-1→L (79.37%)
	S3	3.32	0.0625	373.76	H→L+1 (63.97%)

[a]H and L represent the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively.

Table S6. The S1/S0 difference of twisting angles which are defined as $\Delta\theta=|\theta(S1)-\theta(S0)|$.

Species	$\Delta\theta_{C10\text{-}C11\text{-}C12}$ / °	Emission peak / nm
1-H	0.2085	441.83
1-CH_3	0.2111	443.82
1-OH	0.7941	464.60
1-OCH_3	0.7269	471.83
1-NH_2	1.0353	489.14
1-F	0.3918	450.97
1-CN	1.0143	470.61
1-NO_2	2.3429	548.94

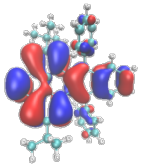
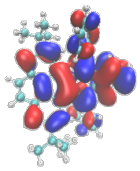
Table S7. Second-order perturbation theory analysis of the Fock matrix based on NBO for 1-H and its derivatives.

Species	Donor	Type	Acceptor	Type	E(2) / kcal/mol
1-H	C11-H82	σ	C10-C16	σ*	4.89
	C10-C16	σ	C11-H82	σ*	2.40
1-CH_3	C82-H84	σ	C11-C12	σ*	4.50
	C10-C16	σ	C11-C82	σ*	3.71
1-OH	O82	n	C10-C11	π*	28.02
	C12-C13	σ	C11-O82	σ*	3.69
1-OCH_3	O82	n	C10-C11	π*	27.92
	C12-C13	σ	C11-O82	σ*	4.26
1-NH_2	N82	n	C10-C11	π*	27.74
	C10-C16	σ	C11-N82	σ*	3.82
1-F	F82	n	C10-C11	π*	19.27
	C10-C16	σ	C11-F82	σ*	4.23
1-CN	C11-C12	π*	C82-N83	π*	25.29
	N83	n	C11-C82	σ*	11.80
1-NO_2	C11-C12	π	N82-O83	π*	26.87
	N82-O83	π*	C11-C12	π*	20.52

Table S8. The optimized twisting angles (θ1, θ2, θ3, θ4 and θ5 in degrees, see in Scheme 1a) and bond lengths (l1, l2, l3, l4 and l5 in Å) of 1-H and its derivatives in their S1 and T2 states.

Species	θ1/θ2	θ3/θ4	θ5	l1/l2	l3/l4	l5
			S1			
1-H	56.7807/56.7693	3.6831/3.6874	0.5541	1.4847/1.4847	1.5402/1.5402	1.0843
1-CH_3	58.5405/54.0585	2.7675/4.4571	0.7053	1.4865/1.4804	1.5403/1.5405	1.5069
1-OH	56.2207/55.5748	2.2031/4.5427	1.5823	1.4823/1.4822	1.5408/1.5405	1.3585
1-OCH_3	55.2923/55.9075	2.2895/4.4219	1.4872	1.4803/1.4827	1.5411/1.5405	1.3542
1-NH_2	55.0262/57.8282	2.0336/4.1674	2.6240	1.4794/1.4873	1.5417/1.5404	1.3658
1-F	59.2318/54.1015	2.6388/4.6778	0.9789	1.4876/1.4796	1.5399/1.5405	1.3538
1-CN	55.6153/60.3218	2.6891/4.6248	0.4240	1.4825/1.4905	1.5401/1.5395	1.4210
1-NO_2	53.1447/64.6517	2.5264/4.5512	1.4494	1.4822/1.4960	1.5398/1.5382	1.4237
			T2			
1-H	56.6928/56.6941	3.1179/3.1194	0.9483	1.4853/1.4853	1.5407/1.5407	1.0838
1-CH_3	57.0338/56.5164	3.0944/3.1899	0.3573	1.4857/1.4853	1.5408/1.5407	1.5060
1-OH	57.6243/57.2539	2.934/3.3169	1.1754	1.4874/1.4869	1.5408/1.5407	1.3603
1-OCH_3	57.4559/57.4035	2.9907/3.1322	0.9485	1.4869/1.4870	1.5409/1.5407	1.3578
1-NH_2	58.0731/58.1223	2.8200/3.1932	3.0258	1.4888/1.4891	1.5410/1.5405	1.3723
1-F	57.5082/56.4739	2.8998/3.2659	1.1351	1.4866/1.4852	1.5407/1.5406	1.3510
1-CN	55.2436/57.7412	2.9993/3.1205	1.0409	1.4834/1.4874	1.5403/1.5401	1.4222
1-NO_2	54.4503/58.9637	2.8029/3.5710	1.6234	1.4829/1.4875	1.5401/1.5398	1.4469

Table S9. Hole and electron NTOs for the optimized S1 and T2 states of 1-H, 1-CH_3 and 1-OH.

Species	Hole	Electron
1-H	Optimized S1	
		
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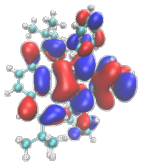
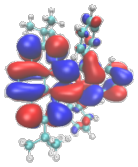
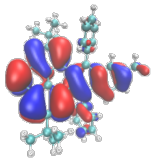
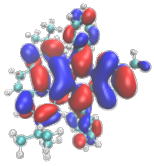
		
1-CH_3	Optimized S1	
		
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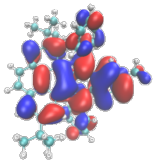
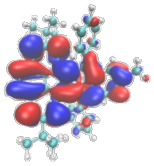
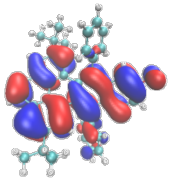
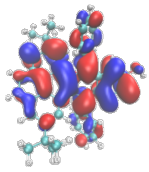
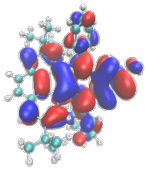
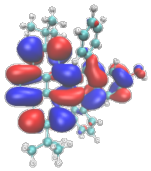
		
1-OH	Optimized S1	
		
	Optimized T2	
		

Table S10. Hole and electron NTOs for the optimized S1 and T2 states of 1-OCH_3, 1-NH_2, and 1-F.

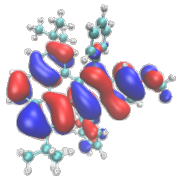
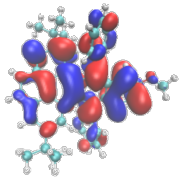
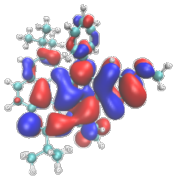
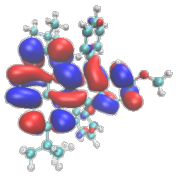
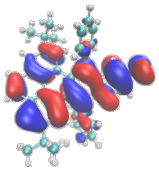
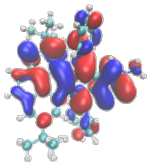
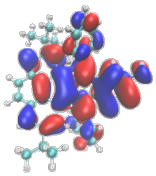
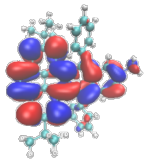
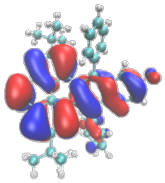
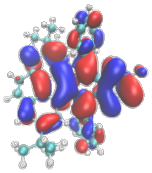
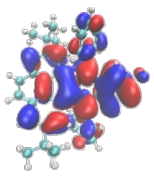
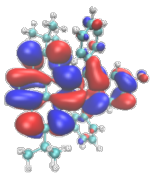
Species	Hole	Electron
1-OCH_3	Optimized S1	
		
	Optimized T2	
		
1-NH_2	Optimized S1	
		
	Optimized T2	
		
1-F	Optimized S1	
		
	Optimized T2	
		

Table S11. Hole and electron NTOs for the optimized S1 and T2 states of 1-CN and 1-NO_2.

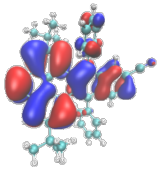
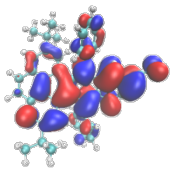
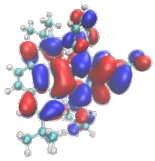
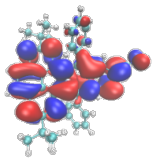
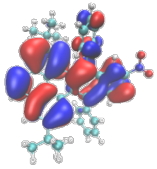
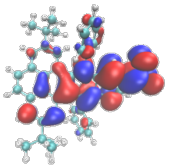
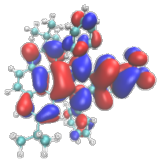
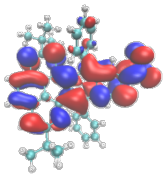
Species	Hole	Electron
1-CN	Optimized S1	
		
	Optimized T2	
		
1-NO_2	Optimized S1	
		
	Optimized T2	
		

Table S12. Intra-molecular hole and electron mobilities of 1-H and its derivatives.

Species	μ_h / $cm^2 \cdot V^{-1} \cdot s^{-1}$	μ_e / $cm^2 \cdot V^{-1} \cdot s^{-1}$
1-H	0.12	10.73
1-CH_3	0.36	7.88
1-OH	2.88	9.18
1-OCH_3	4.16	10.70
1-NH_2	3.35	4.94
1-F	0.38	10.75
1-CN	0.67	23.37
1-NO_2	1.17	20.82

Table S13. The inter-molecular carrier mobilities of 1-H and its derivatives in different stacking patterns.

Species	Stacking patterns	[a]r / Å	μ_e / $cm^2V^{-1}s^{-1}$	μ_h / $cm^2V^{-1}s^{-1}$	[b]r / Å	μ_e / $cm^2V^{-1}s^{-1}$	μ_h / $cm^2V^{-1}s^{-1}$	[c]r / Å	μ_e / $cm^2V^{-1}s^{-1}$	μ_h / $cm^2V^{-1}s^{-1}$
1-H	P stacking	4.60	2.70×10^{-3}	6.48×10^{-4}	6.69	5.70×10^{-3}	1.37×10^{-3}	13.64	2.37×10^{-2}	5.70×10^{-3}
1-CH_3		4.43	1.21×10^{-1}	1.28×10^{-1}	6.73	2.80×10^{-1}	2.95×10^{-1}	11.58	8.28×10^{-1}	8.73×10^{-1}
1-OH		4.69	2.88	1.76	6.84	6.12	3.74	12.40	20.09	12.29
1-OCH_3		6.84	1.74×10^{-1}	2.76×10^{-1}	10.43	4.04×10^{-1}	6.42×10^{-1}	16.79	1.05	1.66
1-NH_2		4.85	1.72	1.92	7.18	3.76	4.21	13.93	14.16	15.85
1-F		4.93	6.02×10^{-4}	3.67×10^{-6}	6.88	1.18×10^{-3}	7.17×10^{-6}	14.18	4.99×10^{-3}	3.04×10^{-5}
1-CN		4.92	6.03×10^{-3}	2.58×10^{-4}	7.98	1.59×10^{-2}	6.82×10^{-4}	15.31	5.85×10^{-2}	2.51×10^{-3}
1-NO_2		4.45	2.14×10^{-1}	7.30×10^{-2}	7.57	6.20×10^{-1}	2.11×10^{-1}	14.33	2.22	7.57×10^{-1}
1-H	P1 stacking	4.16	7.21×10^{-2}	5.38×10^{-2}	6.20	1.60×10^{-1}	1.19×10^{-1}	12.57	6.60×10^{-1}	4.92×10^{-1}
1-CH_3		8.93	2.56×10^{-2}	4.70×10^{-2}	11.82	4.49×10^{-2}	8.23×10^{-2}	18.50	1.10×10^{-1}	2.02×10^{-1}
1-OH		4.51	5.38×10^{-1}	8.63×10^{-1}	6.16	1.00	1.61	12.72	4.27	6.86
1-OCH_3		4.90	5.23×10^{-2}	1.12×10^{-1}	7.28	1.15×10^{-1}	2.48×10^{-1}	13.35	3.88×10^{-1}	8.33×10^{-1}
1-NH_2		4.50	4.01×10^{-1}	3.09×10^{-1}	6.16	7.50×10^{-1}	5.77×10^{-1}	12.72	3.20	2.47
1-F		4.88	4.27×10^{-1}	9.46×10^{-2}	6.81	8.30×10^{-1}	1.84×10^{-1}	13.35	3.19	7.07×10^{-1}
1-CN		5.10	4.91	9.84×10^{-1}	8.97	15.17	3.04	15.53	45.49	9.11
1-NO_2		5.00	3.83	1.17	8.16	10.18	3.12	14.72	33.15	10.16
1-H	L stacking	4.72	6.34×10^{-1}	1.06×10^{-2}	5.36	8.18×10^{-1}	1.37×10^{-1}	8.42	2.02	3.39×10^{-1}
1-CH_3		4.43	6.64×10^{-1}	2.16×10^{-1}	5.37	9.74×10^{-1}	3.17×10^{-1}	8.44	2.41	7.83×10^{-1}
1-OH		3.82	1.12	1.03	7.59	4.41	4.05	9.59	7.02	6.45
1-OCH_3		6.38	9.91×10^{-1}	1.42	5.66	7.80×10^{-1}	1.12	10.20	2.53	3.63

1-NH_2		4.40	6.45×10^{-1}	8.54×10^{-1}	6.13	1.25	1.66	8.25	2.27	3.00
1-F		4.69	5.19×10^{-1}	1.61×10^{-1}	5.42	6.93×10^{-1}	2.15×10^{-1}	8.64	1.76	5.45E-01
1-CN		6.83	1.21×10^{-2}	1.31×10^{-1}	6.43	1.07×10^{-2}	1.17×10^{-1}	9.87	2.53×10^{-2}	2.75×10^{-1}
1-NO_2		7.70	9.79×10^{-2}	1.79×10^{-1}	6.67	7.33×10^{-2}	1.34×10^{-1}	10.58	1.85×10^{-1}	3.37×10^{-1}
1-H	L1 stacking	6.34	1.42×10^{-1}	7.71×10^{-2}	7.57	2.03×10^{-1}	1.10×10^{-1}	11.72	4.86×10^{-1}	2.64×10^{-1}
1-CH_3		10.61	5.27×10^{-4}	1.35×10^{-3}	13.50	8.52×10^{-4}	2.19×10^{-3}	21.02	2.07×10^{-3}	5.31×10^{-3}
1-OH		4.33	1.61×10^{-2}	3.55×10^{-2}	7.07	4.28×10^{-2}	9.47×10^{-2}	13.99	1.68×10^{-1}	3.71×10^{-1}
1-OCH_3		4.96	3.18×10^{-1}	4.82×10^{-1}	7.25	6.78×10^{-1}	1.03	14.17	2.59	3.93
1-NH_2		5.14	1.46×10^{-1}	1.91×10^{-1}	7.07	2.76×10^{-1}	3.62×10^{-1}	13.86	1.06	1.39
1-F		4.51	3.11×10^{-1}	1.31×10^{-1}	6.67	6.80×10^{-1}	2.86×10^{-1}	13.71	2.87	1.21
1-CN		5.01	3.51	1.69×10^{-1}	8.98	11.29	5.44×10^{-1}	16.76	39.27	1.89
1-NO_2		5.30	3.55	1.93×10^{-1}	8.14	8.37	4.56×10^{-1}	15.48	30.29	1.65
1-H	V stacking	5.79	3.39×10^{-2}	1.86×10^{-2}	5.27	2.80×10^{-2}	1.53×10^{-2}	9.03	8.24×10^{-2}	4.51×10^{-2}
1-CH_3		6.66	5.76×10^{-1}	1.83×10^{-1}	5.49	3.92×10^{-1}	1.24×10^{-1}	10.64	1.47	4.66×10^{-1}
1-OH		5.01	1.87×10^{-2}	7.18×10^{-2}	5.38	2.16×10^{-2}	8.28×10^{-2}	10.23	7.81×10^{-2}	3.00×10^{-1}
1-OCH_3		4.99	1.66×10^{-2}	5.88×10^{-4}	5.29	1.86×10^{-2}	6.60×10^{-4}	10.34	7.12×10^{-2}	2.53×10^{-3}
1-NH_2		4.61	3.64×10^{-1}	2.47×10^{-1}	5.33	4.86×10^{-2}	3.30×10^{-1}	10.45	1.87	1.27
1-F		4.99	6.90×10^{-4}	1.66×10^{-3}	5.31	7.83×10^{-4}	1.88×10^{-3}	10.38	2.99×10^{-3}	7.18×10^{-3}
1-CN		4.75	9.90×10^{-1}	6.77×10^{-2}	5.52	1.34	9.14×10^{-2}	10.69	5.00	3.42×10^{-1}
1-NO_2		4.43	1.64	7.22×10^{-2}	7.31	4.48	1.97×10^{-1}	12.14	12.33	5.42×10^{-1}
1-H	V1 stacking	9.86	6.49×10^{-1}	1.99×10^{-1}	6.01	2.41×10^{-1}	7.37×10^{-2}	11.70	9.13×10^{-1}	2.79×10^{-1}
1-CH_3		9.85	4.98×10^{-1}	3.78×10^{-1}	6.05	1.88×10^{-1}	1.43×10^{-1}	11.77	7.11×10^{-1}	5.39×10^{-1}
1-OH		9.77	1.92×10^{-1}	2.77×10^{-1}	6.06	7.38×10^{-2}	1.06×10^{-1}	11.84	2.82×10^{-1}	4.07×10^{-1}

1-OCH_3	9.83	2.43×10^{-1}	3.01×10^{-1}	6.05	9.20×10^{-2}	1.14×10^{-1}	11.56	3.36×10^{-1}	4.17×10^{-1}
1-NH_2	9.92	4.19×10^{-1}	2.95×10^{-1}	6.08	1.58×10^{-1}	1.11×10^{-1}	11.82	5.94×10^{-1}	4.19×10^{-1}
1-F	9.91	3.71×10^{-1}	3.61×10^{-1}	5.95	1.34×10^{-1}	1.30×10^{-1}	11.29	482×10^{-1}	4.69×10^{-1}
1-CN	9.62	4.32×10^{-2}	2.77×10^{-1}	5.92	1.64×10^{-2}	1.05×10^{-1}	11.34	6.01×10^{-2}	3.85×10^{-1}
1-NO_2	9.03	4.17×10^{-1}	7.99×10^{-1}	7.19	2.64×10^{-1}	5.06×10^{-1}	11.74	7.06×10^{-1}	1.35

The three distances along with carrier mobilities are listed. [a]The distance between benzene ring and substituent group. [b]The distance between two benzene rings. [c]The distance of the centre of mass of two adjacent molecules. The relative shortest distance is used in Figure 5 and Figure S2-S7.

Table S14. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at P stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	0.16	0.43	18.54	23.33	1.57×10^{10}	6.54×10^{10}
1-CH_3	2.44	3.33	19.51	24.99	3.34×10^{12}	3.17×10^{12}
1-OH	10.40	17.01	22.63	26.70	4.10×10^{13}	6.71×10^{13}
1-OCH_3	2.90	2.76	23.08	26.05	3.03×10^{12}	1.91×10^{12}
1-NH_2	18.00	15.25	31.64	29.78	4.19×10^{13}	3.75×10^{13}
1-F	0.01	0.22	21.25	25.88	7.77×10^{7}	1.27×10^{10}
1-CN	0.11	0.60	20.45	23.27	5.49×10^{9}	1.28×10^{11}
1-NO_2	1.93	6.21	20.29	30.73	1.89×10^{12}	5.55×10^{12}

Table S15. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at P1 stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	1.59	2.48	18.54	23.33	1.60×10^{12}	2.14×10^{12}
1-CH_3	0.74	0.76	19.51	24.99	3.02×10^{11}	1.65×10^{11}
1-OH	7.57	7.65	22.63	26.70	2.17×10^{13}	1.36×10^{13}
1-OCH_3	2.59	2.11	23.08	26.05	2.40×10^{12}	1.12×10^{12}
1-NH_2	7.78	7.96	31.64	29.78	7.82×10^{12}	1.02×10^{13}
1-F	2.13	6.00	21.25	25.88	2.04×10^{12}	9.19×10^{12}
1-CN	6.25	16.62	20.45	23.27	1.94×10^{13}	9.69×10^{13}
1-NO_2	6.89	23.39	20.29	30.73	2.41×10^{13}	7.86×10^{13}

Table S16. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at L stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	1.97	6.48	18.54	23.33	2.45×10^{12}	1.46×10^{13}
1-CH_3	3.18	7.81	19.51	24.99	5.65×10^{12}	1.74×10^{13}
1-OH	9.75	13.02	22.63	26.70	3.61×10^{13}	3.92×10^{13}
1-OCH_3	7.06	7.06	23.08	26.05	1.79×10^{13}	1.25×10^{13}
1-NH_2	13.25	10.32	31.64	29.78	2.26×10^{13}	1.71×10^{13}
1-F	2.89	6.89	21.25	25.88	3.75×10^{12}	1.21×10^{13}
1-CN	1.71	0.62	20.45	23.27	1.45×10^{12}	1.34×10^{11}
1-NO_2	1.75	2.43	20.29	30.73	1.55×10^{12}	8.47×10^{11}

Table S17. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at L1 stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	1.25	2.28	18.54	23.33	9.84×10^{11}	1.82×10^{12}
1-CH_3	0.11	0.09	19.51	24.99	6.17×10^{9}	2.40×10^{9}
1-OH	1.60	1.38	22.63	26.70	9.72×10^{11}	4.40×10^{11}
1-OCH_3	5.29	5.15	23.08	26.05	1.00×10^{13}	6.63×10^{12}
1-NH_2	5.37	4.20	31.64	29.78	3.72×10^{12}	2.83×10^{12}
1-F	2.70	5.54	21.25	25.88	3.29×10^{12}	7.84×10^{12}
1-CN	2.64	14.31	20.45	23.27	3.46×10^{12}	7.18×10^{13}
1-NO_2	2.64	21.25	20.29	30.73	3.53×10^{12}	6.49×10^{13}

Table S18. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at V stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	0.67	1.22	18.54	23.33	2.84×10^{11}	5.19×10^{11}
1-CH_3	1.94	4.84	19.51	24.99	2.11×10^{12}	6.67×10^{12}
1-OH	1.97	1.29	22.63	26.70	1.47×10^{12}	3.83×10^{11}
1-OCH_3	0.18	1.17	23.08	26.05	1.21×10^{10}	3.42×10^{11}
1-NH_2	6.80	7.40	31.64	29.78	5.97×10^{12}	8.80×10^{12}
1-F	0.28	0.24	21.25	25.88	3.42×10^{10}	1.43×10^{10}
1-CN	1.76	8.01	20.45	23.27	1.54×10^{12}	2.25×10^{13}
1-NO_2	1.93	17.30	20.29	30.73	1.89×10^{12}	4.30×10^{13}

Table S19. The electronic coupling terms, reorganization energies and transport rate constants of 1-H and its derivatives at V1 stacking pattern.

Species	V_h / kJ/mol	V_e / kJ/mol	λ_h / kJ/mol	λ_e / kJ/mol	k_h / s^{-1}	k_e / s^{-1}
1-H	1.29	3.14	18.54	23.33	1.05×10^{12}	3.42×10^{12}
1-CH_3	1.89	3.05	19.51	24.99	2.00×10^{12}	2.64×10^{12}
1-OH	1.98	2.11	22.63	26.70	1.49×10^{12}	1.03×10^{12}
1-OCH_3	2.11	2.27	23.08	26.05	1.60×10^{12}	1.29×10^{12}
1-NH_2	3.45	3.69	31.64	29.78	1.54×10^{12}	2.18×10^{12}
1-F	2.05	2.76	21.25	25.88	1.89×10^{12}	1.94×10^{12}
1-CN	1.76	0.83	20.45	23.27	1.54×10^{12}	2.40×10^{11}
1-NO_2	3.15	4.28	20.29	30.73	5.03×10^{12}	2.63×10^{12}

Table S20. Cartesian coordinates for the optimized species at B3LYP/6-311G** level.

1-H
Energy (with Zero-point Energy correction) = -1700.034584 (-1699.351007) Hartree
Free energy (298 K) = -1699.418396 Hartree
Zero number of imaginary frequency
0 1

C	-1.36459900	1.69870100	0.40404000
C	-0.66011000	2.93499800	0.27772500
C	0.66006100	2.93498600	-0.27790500
C	1.36453800	1.69867700	-0.40416000
H	-2.19532400	4.19977700	1.13824800
C	-1.23931500	4.18743800	0.63490500
C	1.23926700	4.18741300	-0.63512900
C	0.61789100	5.37458800	-0.34085900
C	-0.61793900	5.37460200	0.34059100
H	2.19527300	4.19973600	-1.13847600
C	-3.45417100	-2.04513300	-0.79767000
C	-2.77833600	-0.83974100	-0.52562000
C	-1.43409800	-0.78073900	-0.15392300
C	-0.70464900	-1.99971600	-0.12021100
C	-1.38398600	-3.23151500	-0.31534600
C	-2.74903500	-3.22927500	-0.65163800
C	-0.71931000	0.49639300	0.08575900
C	0.70462100	-1.99969500	0.12030600
C	1.43404200	-0.78070200	0.15392600
C	0.71923300	0.49639200	-0.08584200
C	2.77829000	-0.83964000	0.52558900
H	3.32729800	0.08138600	0.62892500
C	3.45416400	-2.04499400	0.79770500
C	2.74905100	-3.22916400	0.65177300
C	1.38399400	-3.23146200	0.31551100
C	0.65862600	-4.45861200	0.16409700
C	-0.65858900	-4.45863700	-0.16384700
H	-1.19279200	-5.39301200	-0.30158000
H	1.19285200	-5.39296500	0.30188200
H	-3.32736500	0.08126000	-0.62905200
H	-3.22965600	-4.18602500	-0.81098100
H	3.22970200	-4.18589200	0.81116100
C	4.93182800	-2.00626500	1.22947600

C	-4.93181600	-2.00647500	-1.22951200
C	2.75541500	1.74968600	-0.95674700
C	3.79199300	2.43292000	-0.30420000
C	3.02557200	1.16501700	-2.20023600
C	5.05859200	2.52456700	-0.87590200
H	3.60148700	2.89281500	0.65919700
C	4.29027900	1.26066200	-2.77540700
H	2.23271000	0.63917400	-2.71942300
C	5.31165700	1.94147000	-2.11651200
H	5.84708400	3.05437100	-0.35275000
H	4.47577800	0.80554000	-3.74197900
H	6.29592600	2.01700300	-2.56464900
C	-2.75543800	1.74978500	0.95671400
C	-3.02555100	1.16512100	2.20021500
C	-3.79199400	2.43315700	0.30427700
C	-4.29020200	1.26088100	2.77549000
H	-2.23269800	0.63919200	2.71932700
C	-5.05853600	2.52492400	0.87608600
H	-3.60151200	2.89307600	-0.65911400
C	-5.31156200	1.94181400	2.11669800
H	-4.47566800	0.80575600	3.74206800
H	-5.84701200	3.05483300	0.35301700
H	-6.29578600	2.01744000	2.56491900
H	1.08416500	6.31294600	-0.61958400
H	-1.08421400	6.31297000	0.61928000
C	5.47472200	-3.40534800	1.57447900
H	6.51717700	-3.32399100	1.89386000
H	4.91326900	-3.87009700	2.38969100
H	5.44841400	-4.07728400	0.71239900
C	5.78846200	-1.42590300	0.08124500
H	5.71114000	-2.04981000	-0.81353300
H	5.47611200	-0.41602400	-0.18909600
H	6.84180300	-1.38525500	0.37723100
C	5.08297800	-1.11514800	2.48428300
H	4.48200700	-1.50125400	3.31220200
H	6.12893700	-1.09060600	2.80533700
H	4.77101600	-0.08602700	2.29481800
C	-5.47461000	-3.40558000	-1.57458900
H	-6.51706000	-3.32427700	-1.89399900
H	-4.91310300	-3.87026000	-2.38980200
H	-5.44828500	-4.07754900	-0.71253600

C	-5.08295400	-1.11532500	-2.48429800
H	-4.48192600	-1.50137500	-3.31220200
H	-6.12889900	-1.09082400	-2.80539800
H	-4.77105000	-0.08619500	-2.29478300
C	-5.78854500	-1.42620600	-0.08130600
H	-5.71122800	-2.05013600	0.81345600
H	-5.47627500	-0.41631600	0.18908300
H	-6.84187300	-1.38561600	-0.37734400

1-CH_3
Energy (with Zero-point Energy correction) = -1739.362765 (-1738.651944) Hartree
Free energy (298 K) = -1738.721546 Hartree
Zero number of imaginary frequency
0 1

C	-1.32102400	1.58165900	0.45089100
C	-0.55309900	2.77995200	0.35031900
C	0.76724700	2.72600600	-0.19742100
C	1.40771900	1.45833100	-0.34564300
H	-2.01852000	4.11517400	1.22823400
C	-1.06300000	4.05694400	0.72683000
C	1.41216200	3.95426600	-0.52705500
C	0.86775000	5.17939100	-0.22298300
C	-0.37667300	5.21098000	0.45753600
H	2.37108300	3.91970200	-1.02537800
C	-3.59883900	-2.02448300	-0.82711100
C	-2.86248300	-0.86184000	-0.52782000
C	-1.51696000	-0.87983200	-0.15581200
C	-0.85126400	-2.13527100	-0.14964900
C	-1.59253900	-3.32590600	-0.37341500
C	-2.95522800	-3.24628100	-0.70948600
C	-0.73755300	0.35292000	0.11135200
C	0.55552200	-2.21290700	0.09242900
C	1.34641900	-1.03390700	0.15557300
C	0.69901500	0.28343900	-0.05672900
C	2.68460800	-1.17074400	0.52910900
H	3.27970700	-0.28185700	0.65523800
C	3.29672500	-2.41507500	0.77507800
C	2.53235100	-3.55781900	0.60008400
C	1.17026400	-3.48216800	0.26071800
C	0.38344400	-4.66672700	0.07981300
C	-0.93119300	-4.59173400	-0.24977500

H	-1.51224100	-5.49410700	-0.40960200
H	0.86881400	-5.63014300	0.19678900
H	-3.36382800	0.08807700	-0.60950600
H	-3.48381700	-4.17328300	-0.89109600
H	2.96254500	-4.54140900	0.73866800
C	4.77312100	-2.46263700	1.21054400
C	-5.07278400	-1.90057100	-1.25579700
C	2.80250300	1.44914900	-0.89102400
C	3.87022500	2.05981400	-0.21701600
C	3.04849400	0.88298300	-2.14796500
C	5.14307800	2.09876700	-0.78076000
H	3.69858300	2.50478800	0.75688800
C	4.31972200	0.92604500	-2.71526800
H	2.23188300	0.41306400	-2.68373400
C	5.37201800	1.53472800	-2.03487900
H	5.95565600	2.57231500	-0.24071400
H	4.48628800	0.48617400	-3.69231600
H	6.36147500	1.56908500	-2.47663500
C	-2.70898300	1.69563600	1.00120600
C	-3.01442300	1.10219300	2.23234900
C	-3.70535900	2.44588600	0.35972400
C	-4.27413300	1.25439400	2.80625200
H	-2.25266800	0.52442000	2.74283500
C	-4.96724900	2.59420900	0.93002100
H	-3.48727200	2.91308200	-0.59427300
C	-5.25542300	2.00160400	2.15837900
H	-4.48711000	0.79112300	3.76325600
H	-5.72453800	3.17533700	0.41530300
H	-6.23580100	2.12093200	2.60554600
H	-0.79707900	6.16651100	0.75544900
C	5.24034200	-3.89472900	1.53008000
H	6.28426600	-3.87449100	1.85439300
H	4.65161600	-4.34489300	2.33416600
H	5.18257600	-4.54767300	0.65504300
C	5.66240400	-1.90694900	0.07501400
H	5.55456800	-2.50896300	-0.83153200
H	5.40428900	-0.87716200	-0.17665700
H	6.71566400	-1.92756700	0.37345000
C	4.96789200	-1.60459900	2.48226900
H	4.34470200	-1.97352100	3.30156100
H	6.01271700	-1.64205000	2.80581000

H	4.71201100	-0.55689000	2.31172300
C	-5.68497100	-3.26113500	-1.63708300
H	-6.72185400	-3.11931500	-1.95354600
H	-5.14684700	-3.73189100	-2.46449500
H	-5.69302000	-3.95597700	-0.79299100
C	-5.17968300	-0.96996500	-2.48620100
H	-4.59882600	-1.36330500	-3.32500700
H	-6.22319600	-0.88481700	-2.80486900
H	-4.81685700	0.03690200	-2.26983300
C	-5.89907600	-1.30892700	-0.09119000
H	-5.85327200	-1.95992000	0.78630400
H	-5.53590200	-0.32383100	0.20583500
H	-6.94906700	-1.20710900	-0.38442700
C	1.56484600	6.46742600	-0.58178000
H	1.74559900	7.08000700	0.30760400
H	2.52603700	6.28045200	-1.06388700
H	0.95604800	7.06794000	-1.26586600

1-OH

Energy (with Zero-point Energy correction) = -1775.277716 (-1774.590256) Hartree

Free energy (298 K) = -1774.659039 Hartree

Zero number of imaginary frequency

0 1

C	-1.32786900	1.57886200	0.44161800
C	-0.56784700	2.78265000	0.33815500
C	0.75580000	2.73960600	-0.20992000
C	1.40279600	1.47257500	-0.35650200
H	-2.04812900	4.10546600	1.20799700
C	-1.09063900	4.05312000	0.71030200
C	1.39866300	3.96302800	-0.53720400
C	0.82647400	5.17314100	-0.22549300
C	-0.41708000	5.21699500	0.44462900
H	2.36410300	3.96599700	-1.02071100
C	-3.57980200	-2.05150100	-0.81829500
C	-2.85260200	-0.88123700	-0.52567900
C	-1.50673000	-0.88604700	-0.15459400
C	-0.83103200	-2.13617000	-0.14327600
C	-1.56246100	-3.33384900	-0.36104000
C	-2.92627600	-3.26740300	-0.69592500
C	-0.73700000	0.35364000	0.10771400
C	0.57657100	-2.20101800	0.09874100

C	1.35819700	-1.01562200	0.15657700
C	0.70114600	0.29632400	-0.06212200
C	2.69714800	-1.13963500	0.53134800
H	3.28486600	-0.24517500	0.65275900
C	3.31942900	-2.37773900	0.78326000
C	2.56438400	-3.52729100	0.61292600
C	1.20174100	-3.46436200	0.27282400
C	0.42482600	-4.65619600	0.09722400
C	-0.89049800	-4.59354600	-0.23222500
H	-1.46407400	-5.50142100	-0.38787900
H	0.91823600	-5.61502300	0.21824600
H	-3.36189800	0.06398500	-0.61260100
H	-3.44722800	-4.19962000	-0.87278100
H	3.00258800	-4.50675300	0.75579000
C	4.79601900	-2.41112600	1.21915300
C	-5.05503300	-1.94153800	-1.24644300
C	2.79539100	1.46999400	-0.90688900
C	3.86214300	2.09220800	-0.24201000
C	3.03932000	0.89741600	-2.16140000
C	5.13197400	2.13571000	-0.81198700
H	3.69251600	2.54391100	0.72908300
C	4.30769700	0.94431200	-2.73457000
H	2.22314800	0.41944800	-2.69068600
C	5.35898000	1.56435000	-2.06307100
H	5.94330100	2.61989800	-0.27967700
H	4.47250400	0.49944200	-3.70965400
H	6.34597800	1.60307900	-2.50992400
C	-2.71739400	1.68708500	0.98925300
C	-3.01987600	1.10095100	2.22459600
C	-3.71845400	2.42527600	0.34097800
C	-4.28121100	1.24884800	2.79609300
H	-2.25465600	0.53200400	2.73972900
C	-4.98198500	2.56920300	0.90892300
H	-3.50317900	2.88500400	-0.61734400
C	-5.26708400	1.98424800	2.14165000
H	-4.49202600	0.79114000	3.75623700
H	-5.74322700	3.14003400	0.38851500
H	-6.24883500	2.09974600	2.58679300
H	-0.84137400	6.17281200	0.73927800
C	5.27502900	-3.83795200	1.54468700
H	6.31872300	-3.80768300	1.86895300

H	4.68999200	-4.28965400	2.35062600
H	5.22276600	-4.49497300	0.67235100
C	5.68084500	-1.85263600	0.08150800
H	5.57827700	-2.45924800	-0.82257700
H	5.41429200	-0.82608800	-0.17453400
H	6.73415500	-1.86323700	0.38028000
C	4.98321100	-1.54621700	2.48737300
H	4.36297100	-1.91703100	3.30807400
H	6.02825000	-1.57348700	2.81123000
H	4.71858500	-0.50142400	2.31237500
C	-5.65749600	-3.30918500	-1.61771100
H	-6.69581000	-3.17732000	-1.93384500
H	-5.11684600	-3.78147800	-2.44257400
H	-5.65914000	-3.99828100	-0.76889100
C	-5.16986600	-1.02036800	-2.48322800
H	-4.58677900	-1.41532000	-3.31971000
H	-6.21424100	-0.94504300	-2.80163600
H	-4.81401500	-0.00944600	-2.27422500
C	-5.88497500	-1.34808100	-0.08536200
H	-5.83348500	-1.99256800	0.79661000
H	-5.52908600	-0.35819000	0.20446200
H	-6.93595600	-1.25632600	-0.37842700
O	1.50065200	6.31364400	-0.56191900
H	0.98206500	7.07873000	-0.29387600

1-OCH_3

Energy (with Zero-point Energy correction) = -1814.587124 (-1813.871451) Hartree

Free energy (298 K) = -1813.942261 Hartree

Zero number of imaginary frequency

0 1

C	-1.26569500	1.46084800	0.46006100
C	-0.43279900	2.61755400	0.36435200
C	0.88547900	2.49668000	-0.18540000
C	1.45441000	1.19196500	-0.34093300
H	-1.82631100	4.02292000	1.23916200
C	-0.87328400	3.91419200	0.74173400
C	1.59876700	3.67896900	-0.50165300
C	1.10611600	4.92733100	-0.18533700
C	-0.13356600	5.04319300	0.48488900
H	2.56389900	3.62869800	-0.98331100
C	-3.73541400	-2.01387300	-0.83013600

C	-2.93805400	-0.89297200	-0.52697200
C	-1.59514000	-0.98318800	-0.15630000
C	-0.99728500	-2.27246000	-0.15585900
C	-1.80039800	-3.42109200	-0.38478800
C	-3.15740700	-3.26841400	-0.71946900
C	-0.75127300	0.20521200	0.11675400
C	0.40348500	-2.42584700	0.08693000
C	1.25645400	-1.29137300	0.15534200
C	0.68202600	0.06046100	-0.05478200
C	2.58440800	-1.50057200	0.53108100
H	3.22602900	-0.64497400	0.65996000
C	3.12876200	-2.77665400	0.77438300
C	2.30489300	-3.87612600	0.59339800
C	0.94942700	-3.72659900	0.25134900
C	0.10118900	-4.86692000	0.06420500
C	-1.20715000	-4.72072800	-0.26657800
H	-1.83509500	-5.59028400	-0.43098400
H	0.53455500	-5.85525600	0.17758300
H	-3.38876500	0.08225200	-0.60467300
H	-3.73410900	-4.16542800	-0.90512300
H	2.68145400	-4.88188100	0.72920300
C	4.59952600	-2.90430900	1.21263100
C	-5.20138000	-1.80998900	-1.25561800
C	2.84525900	1.10868500	-0.88878800
C	3.94620400	1.66110800	-0.21790400
C	3.05726400	0.52999400	-2.14632300
C	5.21781600	1.63070200	-0.78473700
H	3.80181600	2.11624200	0.75564900
C	4.32759700	0.50324400	-2.71641700
H	2.21492300	0.10553700	-2.68020000
C	5.41293600	1.05410400	-2.03879700
H	6.05576400	2.06120500	-0.24752800
H	4.46758800	0.05505300	-3.69386900
H	6.40163900	1.03525800	-2.48318700
C	-2.64626200	1.65105700	1.00771700
C	-2.98553500	1.07590200	2.23866300
C	-3.59940400	2.45405300	0.36420500
C	-4.23615500	1.29657700	2.81025500
H	-2.25710500	0.45757800	2.75022500
C	-4.85252400	2.67073100	0.93208000
H	-3.35494300	2.90711000	-0.59025600

C	-5.17449000	2.09533800	2.16025500
H	-4.47570700	0.84582500	3.76695700
H	-5.57674400	3.29088700	0.41526800
H	-6.14793400	2.26739500	2.60540100
H	-0.51484100	6.00823400	0.79037600
C	4.98812600	-4.36001600	1.53071500
H	6.03080400	-4.39666900	1.85765000
H	4.37384200	-4.77919100	2.33245600
H	4.89754700	-5.00739300	0.65432200
C	5.51968900	-2.39549700	0.07973600
H	5.38164700	-2.98965400	-0.82789300
H	5.31762700	-1.35305200	-0.17103200
H	6.56970900	-2.47288100	0.38029400
C	4.83764100	-2.05993200	2.48608900
H	4.19397400	-2.39609200	3.30367200
H	5.87833900	-2.15389800	2.81144000
H	4.63875200	-0.99977100	2.31664600
C	-5.88515700	-3.13421600	-1.64321500
H	-6.91357200	-2.93616000	-1.95719000
H	-5.37369500	-3.62816800	-2.47399600
H	-5.92863200	-3.83227600	-0.80287400
C	-5.26127300	-0.86833000	-2.48080100
H	-4.70284100	-1.28685500	-3.32263100
H	-6.29938400	-0.72713100	-2.79732200
H	-4.84606500	0.11701400	-2.25965200
C	-5.99350400	-1.18208500	-0.08629200
H	-5.98096500	-1.83966000	0.78739900
H	-5.57782100	-0.21949200	0.21562000
H	-7.03706900	-1.02287300	-0.37700200
O	1.88450500	5.99227400	-0.53659600
C	1.42816900	7.30334200	-0.23647000
H	0.47450100	7.52300500	-0.72939800
H	1.32387400	7.45935500	0.84321300
H	2.19231600	7.97696700	-0.62113300

1-NH_2

Energy (with Zero-point Energy correction) = -1755.408791 (-1754.708778) Hartree

Free energy (298 K) = -1754.777655 Hartree

Zero number of imaginary frequency

0 1

C	-1.32370500	1.58085600	0.44447900

C	-0.56113700	2.78025600	0.34108400
C	0.76216700	2.73536800	-0.20537500
C	1.40570900	1.46642400	-0.34759800
H	-2.03243000	4.11352400	1.21227200
C	-1.07683800	4.05677200	0.71088700
C	1.40363200	3.95779200	-0.53947900
C	0.84435600	5.18422100	-0.23774700
C	-0.40188200	5.21572700	0.44380600
H	2.36941000	3.93120400	-1.02558400
C	-3.59108800	-2.03873500	-0.82216100
C	-2.85946200	-0.87271200	-0.52443800
C	-1.51230600	-0.88333400	-0.15675600
C	-0.84129200	-2.13635800	-0.15435300
C	-1.57707000	-3.33029200	-0.37870600
C	-2.94135800	-3.25776300	-0.71000000
C	-0.73765900	0.35162700	0.10948800
C	0.56606800	-2.20749200	0.08674300
C	1.35144500	-1.02477800	0.15318000
C	0.69919500	0.29046200	-0.06008900
C	2.68926700	-1.15616000	0.53012700
H	3.27937600	-0.26451700	0.66005500
C	3.30709600	-2.39790000	0.77475400
C	2.54893500	-3.54396600	0.59479400
C	1.18709400	-3.47409300	0.25316400
C	0.40633200	-4.66215800	0.06936100
C	-0.90893300	-4.59292600	-0.25900900
H	-1.48563900	-5.49790700	-0.42013100
H	0.89660100	-5.62341900	0.18400000
H	-3.36610800	0.07453800	-0.60427500
H	-3.46563200	-4.18719500	-0.89161200
H	2.98358900	-4.52585400	0.73182300
C	4.78252300	-2.43915200	1.21419000
C	-5.06750000	-1.92128600	-1.24449500
C	2.80221800	1.46247700	-0.88851600
C	3.86570700	2.07692900	-0.21063900
C	3.05527700	0.90010500	-2.14586800
C	5.14021100	2.12218700	-0.77020700
H	3.68874200	2.52027000	0.76304500
C	4.32837500	0.94868000	-2.70896100
H	2.24233700	0.42727900	-2.68471900
C	5.37597300	1.56074900	-2.02445200

H	5.94922200	2.59753100	-0.22624100
H	4.50011900	0.50983800	-3.68565300
H	6.36705300	1.59888500	-2.46239100
C	-2.71145700	1.69217600	0.99617100
C	-3.01282000	1.10277000	2.23027000
C	-3.71193800	2.43576700	0.35331100
C	-4.27211100	1.25272700	2.80564800
H	-2.24794400	0.52975700	2.74137600
C	-4.97354800	2.58181800	0.92500600
H	-3.49734000	2.89849500	-0.60368100
C	-5.25742400	1.99350400	2.15638900
H	-4.48179700	0.79252500	3.76487700
H	-5.73420100	3.15723600	0.40873900
H	-6.23760100	2.11072000	2.60460300
H	-0.81946900	6.17063300	0.74706300
C	5.25592600	-3.86957500	1.53216100
H	6.29885600	-3.84490300	1.85947600
H	4.66704500	-4.32423600	2.33359900
H	5.20371600	-4.52101600	0.65564700
C	5.67234500	-1.87684800	0.08237300
H	5.57012700	-2.47775600	-0.82557900
H	5.40949700	-0.84800300	-0.16817700
H	6.72489900	-1.89258100	0.38377100
C	4.96971400	-1.58281800	2.48819300
H	4.34612500	-1.95658300	3.30498700
H	6.01388000	-1.61566200	2.81450800
H	4.70886100	-0.53611300	2.31913600
C	-5.67542500	-3.28433400	-1.62378300
H	-6.71447300	-3.14708700	-1.93530500
H	-5.13892400	-3.75216700	-2.45389500
H	-5.67610200	-3.97965800	-0.78006300
C	-5.18419400	-0.99072300	-2.47404200
H	-4.60513400	-1.38120600	-3.31544100
H	-6.22951300	-0.91011200	-2.78818100
H	-4.82468400	0.01755500	-2.25874200
C	-5.89167100	-1.33393000	-0.07623200
H	-5.83886400	-1.98503300	0.80079100
H	-5.53167500	-0.34732900	0.21960000
H	-6.94348300	-1.23692300	-0.36478300
N	1.50587300	6.38030900	-0.50900600
H	2.22719600	6.32504000	-1.21303000

H	0.91077900	7.18572500	-0.63486800

1-F
Energy (with Zero-point Energy correction) = -1799.299373 (-1798.624152) Hartree
Free energy (298 K) = -1798.692717 Hartree
Zero number of imaginary frequency
0 1

C	-1.32965400	1.58035300	0.44152800
C	-0.57191300	2.78607100	0.33795900
C	0.75221100	2.73878400	-0.20794000
C	1.40204400	1.47597900	-0.35515600
H	-2.05987900	4.10243300	1.20689400
C	-1.10144400	4.05593500	0.71097500
C	1.39499600	3.96660100	-0.53587200
C	0.80241800	5.15312200	-0.21563700
C	-0.43365200	5.22397700	0.44609800
H	2.35983600	3.97915800	-1.02027100
C	-3.57551000	-2.05237700	-0.81928700
C	-2.84976000	-0.88125900	-0.52670700
C	-1.50450800	-0.88516700	-0.15386000
C	-0.82739000	-2.13432800	-0.13980000
C	-1.55774300	-3.33289600	-0.35635800
C	-2.92097300	-3.26744600	-0.69340000
C	-0.73597200	0.35598600	0.10699700
C	0.58006600	-2.19800700	0.10234800
C	1.36086500	-1.01216100	0.15817600
C	0.70185900	0.29826700	-0.05994800
C	2.70075100	-1.13412600	0.53026900
H	3.28809200	-0.23917900	0.64983500
C	3.32437200	-2.37137300	0.78267500
C	2.56957700	-3.52163900	0.61544400
C	1.20638900	-3.46058300	0.27731300
C	0.43027300	-4.65329500	0.10410200
C	-0.88512000	-4.59200600	-0.22521400
H	-1.45808900	-5.50043800	-0.37947000
H	0.92432900	-5.61155500	0.22647500
H	-3.35974500	0.06342300	-0.61499500
H	-3.44118000	-4.20019900	-0.86953400
H	3.00890900	-4.50044500	0.75909300
C	4.80168200	-2.40308900	1.21612100
C	-5.04997600	-1.94451000	-1.25035600

C	2.79381500	1.47743800	-0.90751600
C	3.85940700	2.10226100	-0.24322900
C	3.03690400	0.90730000	-2.16332400
C	5.12798300	2.15150100	-0.81583500
H	3.69091600	2.54977100	0.73010200
C	4.30392000	0.96007300	-2.73877800
H	2.22160200	0.42693100	-2.69174100
C	5.35418800	1.58316500	-2.06834300
H	5.93872400	2.63721500	-0.28415500
H	4.46854100	0.51746100	-3.71484800
H	6.34002100	1.62630400	-2.51720400
C	-2.71943200	1.68493300	0.98936800
C	-3.01923700	1.09846000	2.22513700
C	-3.72255000	2.42007500	0.34088700
C	-4.28063100	1.24340000	2.79721400
H	-2.25226800	0.53218000	2.74062800
C	-4.98600000	2.56098400	0.90960900
H	-3.50928300	2.88057200	-0.61752600
C	-5.26864200	1.97590600	2.14283700
H	-4.48958400	0.78609600	3.75790400
H	-5.74869100	3.13023400	0.38975900
H	-6.25019400	2.08963100	2.58876100
H	-0.83739200	6.18964000	0.72349100
C	5.28317100	-3.82955400	1.53946100
H	6.32746100	-3.79815500	1.86151200
H	4.70064500	-4.28263900	2.34641800
H	5.22997600	-4.48598500	0.66674000
C	5.68382000	-1.84227500	0.07750500
H	5.58065800	-2.44798600	-0.82710100
H	5.41576900	-0.81565500	-0.17687500
H	6.73754300	-1.85187000	0.37456800
C	4.98938000	-1.53900600	2.48483300
H	4.37115600	-1.91153400	3.30624500
H	6.03491500	-1.56485600	2.80698800
H	4.72286200	-0.49440500	2.31134500
C	-5.64956300	-3.31313500	-1.62264100
H	-6.68728000	-3.18273800	-1.94112600
H	-5.10653500	-3.78485100	-2.44627500
H	-5.65244000	-4.00209100	-0.77371100
C	-5.16354200	-1.02358100	-2.48743600
H	-4.57829900	-1.41762200	-3.32282800

H	-6.20733900	-0.94999900	-2.80786000
H	-4.81005300	-0.01191700	-2.27793800
C	-5.88275000	-1.35209900	-0.09076600
H	-5.83210700	-1.99632600	0.79143000
H	-5.52896300	-0.36156200	0.19947100
H	-6.93323000	-1.26190600	-0.38583300
F	1.42620100	6.31365900	-0.52501100

1-CN

Energy (with Zero-point Energy correction) = -1792.300579 (-1791.618345) Hartree

Free energy (298 K) = -1791.688272 Hartree

Zero number of imaginary frequency

0 1

C	-1.26779400	1.55060600	0.48218800
C	-0.43548400	2.70531500	0.39871000
C	0.88124500	2.58180600	-0.15155000
C	1.45488800	1.28370800	-0.31736400
H	-1.82804000	4.09869200	1.30397400
C	-0.87832500	4.00093000	0.79855300
C	1.59163700	3.76882700	-0.47208800
C	1.09709700	5.01446700	-0.14020000
C	-0.14103400	5.12517800	0.54731000
H	2.54433400	3.70115100	-0.97579500
C	-3.73254600	-1.90462300	-0.85663000
C	-2.93518000	-0.78848300	-0.53806300
C	-1.59430600	-0.88678100	-0.16201200
C	-0.99779500	-2.17656400	-0.16785500
C	-1.80255300	-3.32128600	-0.40932700
C	-3.15671900	-3.16103600	-0.75127500
C	-0.75000900	0.29731400	0.12287200
C	0.40084400	-2.33542800	0.07999900
C	1.25603900	-1.20396900	0.16041100
C	0.68267300	0.14862400	-0.03786400
C	2.58356300	-1.41711800	0.53498400
H	3.22705000	-0.56393500	0.67099100
C	3.12456200	-2.69617400	0.76943600
C	2.29791800	-3.79230500	0.57896900
C	0.94344100	-3.63843600	0.23531500
C	0.09317800	-4.77537600	0.03674400
C	-1.21345600	-4.62348900	-0.29805100
H	-1.84278200	-5.49005200	-0.47171300

H	0.52359700	-5.76550100	0.14418000
H	-3.38325500	0.18851700	-0.60816100
H	-3.73488400	-4.05479700	-0.94756400
H	2.67277400	-4.79950000	0.70795900
C	4.59412400	-2.83049800	1.20933600
C	-5.19500200	-1.69493200	-1.29074400
C	2.84582600	1.20618600	-0.86494300
C	3.94351000	1.75963800	-0.18970900
C	3.05876600	0.63325900	-2.12497300
C	5.21518500	1.73804100	-0.75717700
H	3.79863800	2.20674500	0.78765600
C	4.32905300	0.61618300	-2.69488900
H	2.21866400	0.20773300	-2.66144200
C	5.41165900	1.16912500	-2.01423300
H	6.05084600	2.17064700	-0.21861700
H	4.47115800	0.17492900	-3.67499100
H	6.39983500	1.15871500	-2.45962800
C	-2.64799200	1.73158100	1.03413200
C	-2.98423600	1.13932400	2.25766800
C	-3.60171400	2.54238500	0.40168600
C	-4.23417400	1.35188500	2.83361400
H	-2.25504000	0.51526900	2.76117900
C	-4.85394200	2.75091200	0.97441900
H	-3.35955700	3.00886900	-0.54692900
C	-5.17342100	2.15885800	2.19522900
H	-4.47203200	0.88916600	3.78486500
H	-5.57861900	3.37845600	0.46763300
H	-6.14586100	2.32532000	2.64439200
H	-0.49691700	6.10061000	0.85419000
C	4.97997700	-4.29015300	1.51200900
H	6.02196000	-4.33168000	1.84006500
H	4.36439900	-4.71719700	2.30855800
H	4.89021600	-4.92792300	0.62851800
C	5.51708100	-2.31028300	0.08384800
H	5.38019100	-2.89360600	-0.83091300
H	5.31802600	-1.26437700	-0.15503800
H	6.56607700	-2.39301800	0.38575900
C	4.82975500	-2.00019900	2.49251600
H	4.18408100	-2.34446300	3.30506700
H	5.86941300	-2.09892900	2.81913700
H	4.63297600	-0.93781200	2.33446800

C	-5.87714800	-3.01490300	-1.69519700
H	-6.90258500	-2.81251400	-2.01550600
H	-5.36024700	-3.50224100	-2.52651600
H	-5.92885700	-3.72025100	-0.86143400
C	-5.24414300	-0.74198400	-2.50766100
H	-4.68028100	-1.15327800	-3.34938600
H	-6.27956700	-0.59680100	-2.83041300
H	-4.83013700	0.24122600	-2.27473900
C	-5.99426700	-1.07664900	-0.12109200
H	-5.98889500	-1.74181100	0.74686200
H	-5.58029200	-0.11684100	0.19206000
H	-7.03534600	-0.91388500	-0.41791300
C	1.83759200	6.19246900	-0.46961200
N	2.42838900	7.15123800	-0.72934800

1-NO_2

Energy (with Zero-point Energy correction) = -1904.592597 (-1903.906766) Hartree

Free energy (298 K) = -1903.97846 Hartree

Zero number of imaginary frequency

0 1

C	1.52210900	0.90944900	-0.28820300
C	1.11382100	2.26659900	-0.10847200
C	-0.18147800	2.55042000	0.43644300
C	-1.15106200	1.50804100	0.50408400
H	2.91682300	3.20141800	-0.90515500
C	1.97120500	3.35718000	-0.41015400
C	-0.46285400	3.88810200	0.84779700
C	0.41027200	4.91592800	0.61423200
C	1.61497600	4.63267100	-0.05888800
H	-1.39661100	4.09834700	1.34823800
C	2.67945900	-3.25393300	0.77355000
C	2.30291600	-1.91611900	0.54558900
C	1.01325000	-1.53728500	0.16995000
C	0.02382600	-2.55259200	0.08095000
C	0.39879100	-3.91388700	0.23083100
C	1.72266000	-4.23728500	0.57612300
C	0.61342000	-0.12279100	-0.02001600
C	-1.34266200	-2.21887900	-0.17175400
C	-1.77330100	-0.86463300	-0.16261000
C	-0.79008100	0.20281100	0.13524200
C	-3.08842700	-0.59703800	-0.54728400

H	-3.40939900	0.42889600	-0.61642000
C	-4.01707400	-1.60308000	-0.87631100
C	-3.60428700	-2.92225200	-0.77160500
C	-2.28315400	-3.25269000	-0.42249500
C	-1.86241800	-4.61889100	-0.31442300
C	-0.58642100	-4.93456100	0.02430100
H	-0.28379200	-5.97122800	0.12849700
H	-2.59450300	-5.39909200	-0.49455200
H	3.04732700	-1.15035400	0.68725500
H	1.96869200	-5.28402000	0.70025700
H	-4.28896900	-3.73558900	-0.97491700
C	-5.43778100	-1.20988700	-1.32138500
C	4.11962500	-3.57268400	1.21550900
C	-2.50167300	1.85286400	1.05136700
C	-3.34359200	2.78227400	0.42351600
C	-2.91602100	1.29412500	2.26667900
C	-4.56338900	3.13900600	0.99307400
H	-3.03990600	3.22508900	-0.51871600
C	-4.13317600	1.65438800	2.83935300
H	-2.27300600	0.57922300	2.76684100
C	-4.96099800	2.57865300	2.20585500
H	-5.20129000	3.85732400	0.49022500
H	-4.43210100	1.21505900	3.78443300
H	-5.90761600	2.86035100	2.65265400
C	2.89176400	0.66395200	-0.83855900
C	3.02911600	0.07035000	-2.09970100
C	4.05052500	1.07799900	-0.16595100
C	4.28598000	-0.10146300	-2.67310000
H	2.14169300	-0.24805100	-2.63422700
C	5.30827400	0.90155500	-0.73724300
H	3.96488600	1.53852400	0.81207200
C	5.42995800	0.31422300	-1.99503600
H	4.37029900	-0.55510900	-3.65420600
H	6.19178200	1.23006100	-0.20170800
H	6.40808500	0.18446900	-2.44378100
H	0.19578900	5.93013100	0.91850700
C	5.10423400	-3.15753600	0.09864200
H	4.90059500	-3.70935700	-0.82320200
H	5.03681100	-2.09246000	-0.12877600
H	6.13371200	-3.37220000	0.40265800
C	4.32197900	-5.07186700	1.50272100

H	5.35025200	-5.24487900	1.83095600
H	3.65708900	-5.42830900	2.29435000
H	4.15596200	-5.68420700	0.61229400
C	4.44986500	-2.79136200	2.50860200
H	3.76302500	-3.06209900	3.31520500
H	5.46797300	-3.02086300	2.83737300
H	4.38610000	-1.71118800	2.36163500
C	-5.35535300	-0.25996600	-2.53892300
H	-6.36113900	0.01628300	-2.86967000
H	-4.82043900	0.66238600	-2.30308600
H	-4.84245900	-0.74114100	-3.37618700
C	-6.27905200	-2.43288000	-1.73070900
H	-7.26823500	-2.10218100	-2.05810100
H	-5.82257200	-2.98238600	-2.55861200
H	-6.42551500	-3.12537100	-0.89741300
C	-6.16093100	-0.49327600	-0.15832200
H	-6.24635300	-1.15205700	0.71031000
H	-5.63138900	0.40710600	0.15719000
H	-7.17075700	-0.20063100	-0.46328400
N	2.53191500	5.74297000	-0.38003100
O	2.18820300	6.87100300	-0.04596900
O	3.57913500	5.47834600	-0.95757100