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

Supporting Information

How structural factors determine linear and non-linear optical properties of fluorene-containing quadrupolar fluorophores? A theoretical answer

Safa Gam,[abc] Sabri Messaoudi,[bcd] Jean-François Halet*[ae] and Abdou Boucekkine*[a]

[a]*Univ Rennes, CNRS, Institut des Sciences Chimiques de Rennes (ISCR) – UMR 6226, F35000 Rennes, France. E-mail: Abdou.Boucekkine@univ-rennes1.fr*

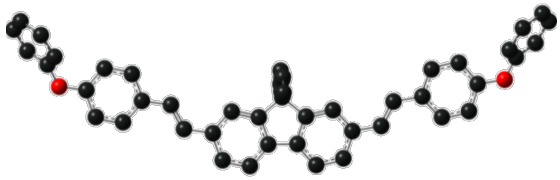
[b]*Faculty of Sciences of Bizerte FSB, University of Carthage, 7021 Jarzouna, Tunisia*

[c]*Laboratory of Materials, Molecules and Applications, IPEST, University of Carthage, Sidi Bou Said Road, B.P. 51, 2070 La Marsa, Tunisia*

[d]*Department of Chemistry, College of Science, Qassim University, Buraidah 51452, Saudi Arabia*

[e]*CNRS – Saint-Gobain – NIMS, IRL 3629, Laboratory for Innovative Key Materials and Structures (LINK), National Institute for Materials Science (NIMS), Tsukuba, 305-0044, Japan. E-mail: Jean-Francois.Halet@univ-rennes1.fr*

Molecule **OPh-PV**



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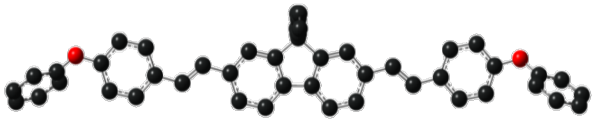

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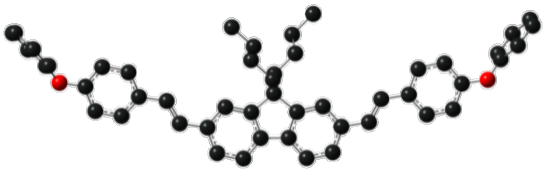

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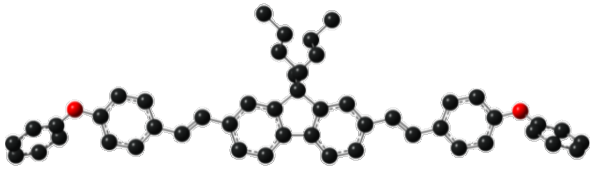
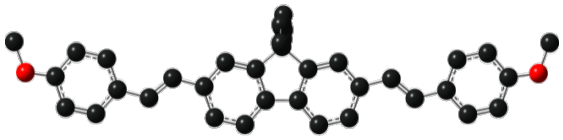


(d)

Molecule **OMe-PV**



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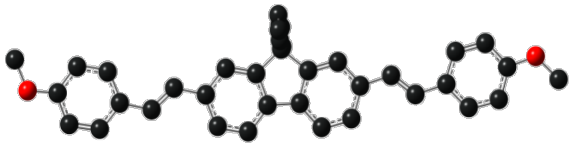

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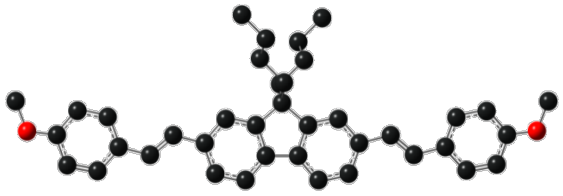

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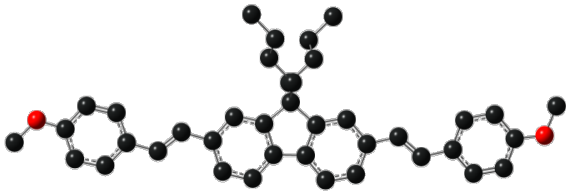

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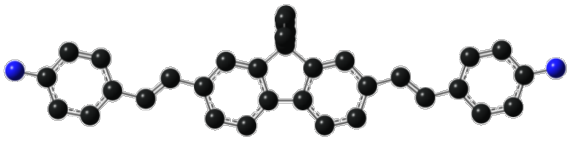
Molecule **NH_2-PV**



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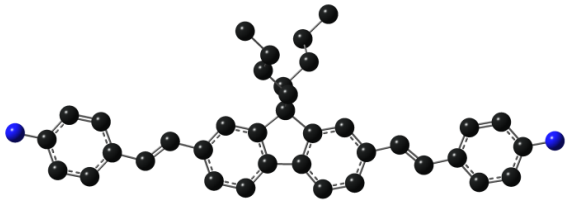

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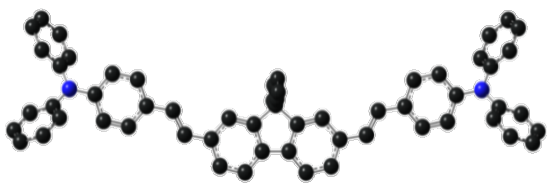
Molecule **NPh_2-PV**



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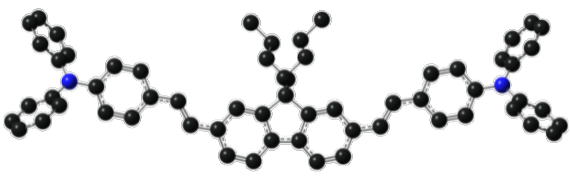

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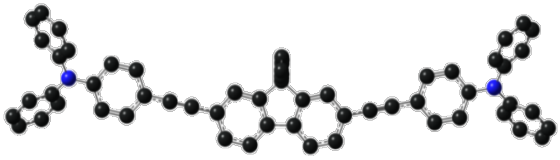
Molecule **NPh_2-PE**



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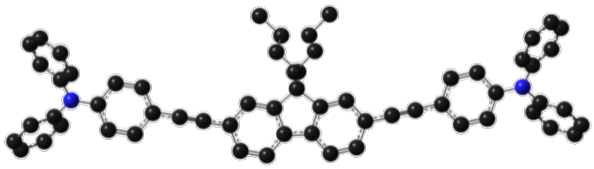
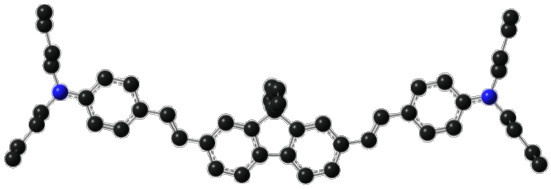


(b)

Molecule **NBu_2-PV**



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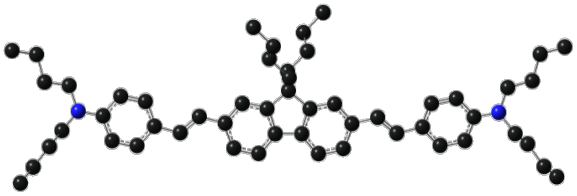
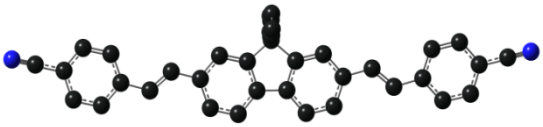


(b)

Molecule **CN-PV**



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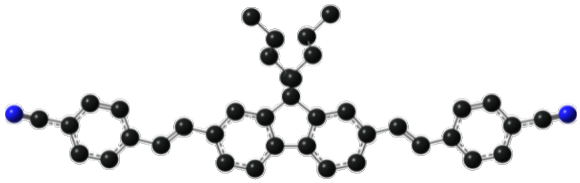
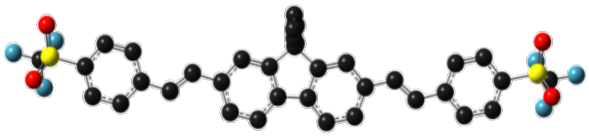


(b)

Molecule **SO_2CF_3-PV**



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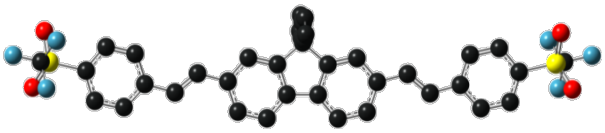

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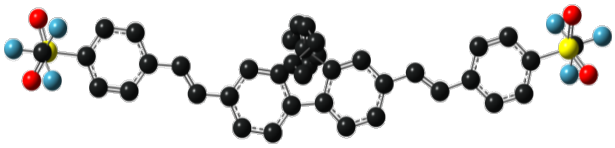

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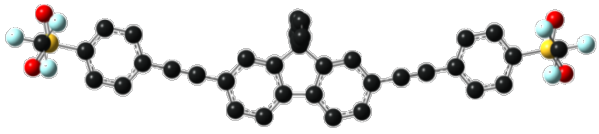
Molecule **SO_2CF_3-PE**



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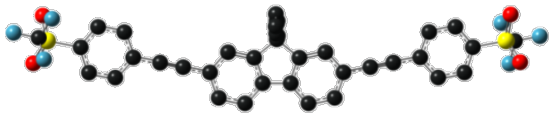

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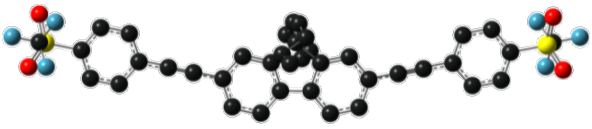

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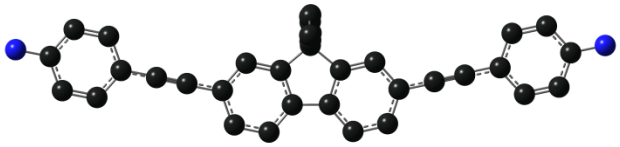
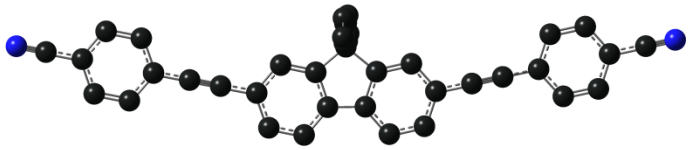
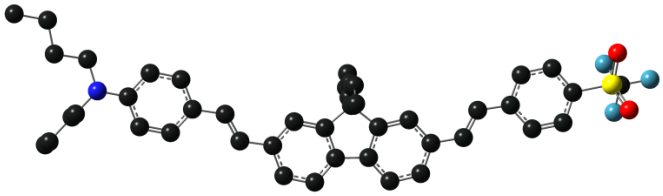
Molecule **NH_2-PE**



Molecule **CN-PE**



Molecule **NBu_2-PV-SO_2CF_3**



Molecule **NPh_2-PE-CPDT**

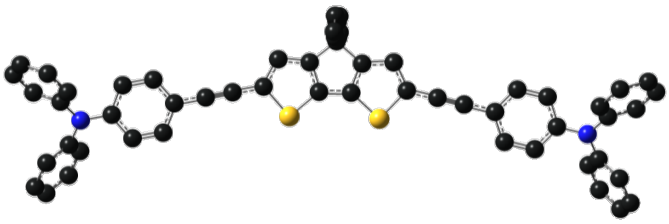
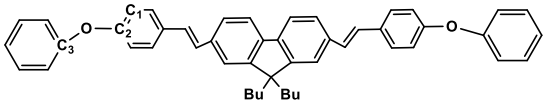


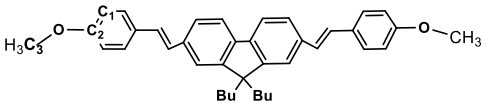
Figure S1 PBE0/6-31+G(d)-optimized geometries in toluene of the different forms of the studied molecules. Hydrogen atoms are omitted for clarity. Black, blue, red, cyan, and yellow spheres are C, N, O, F, and S atoms, respectively.

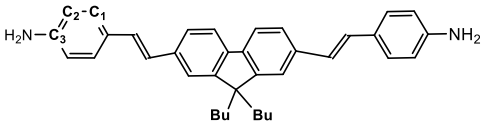
Table S1 Calculated mean deviation from planarity of different geometrical forms of the **X-PV** and **X-PE** series of compounds. See Scheme S1 for the atom numbering

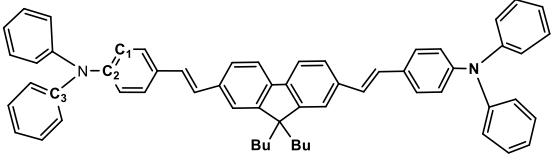
Cmpd	Dihedral angle[a]	Mean deviation (°)
OPh-PV(a)	C_1-C_2-O-C_3	30
OPh-PV(b)	C_1-C_2-O-C_3	30
OPh-PV(c)	C_1-C_2-O-C_3	30
OPh-PV(d)	C_1-C_2-O-C_3	31
OMe-PV(a)	C_1-C_2-O-C_3	0
OMe-PV(b)	C_1-C_2-O-C_3	0
OMe-PV(c)	C_1-C_2-O-C_3	0
OMe-PV(d)	C_1-C_2-O-C_3	0
NH_2-PV(a)	C_1-C_2-C_3-N	3
NH_2-PV(b)	C_1-C_2-C_3-N	3
NPh_2-PV(a)	C_1-C_2-N-C_3	38
NPh_2-PV(b)	C_1-C_2-N-C_3	38
NPh_2-PE(a)	C_1-C_2-N-C_3	36
NPh_2-PE(b)	C_1-C_2-N-C_3	36
NBu_2-PV(a)	C_1-C_2-N-C_3	2
NBu_2-PV(b)	C_1-C_2-N-C_3	3
CN-PV(a)	C_1-C_2-C_3-C_4	0
CN-PV(b)	C_1-C_2-C_3-C_4	0
SO_2CF_3-PV(a)	C_1-C_2-S-C_3	89
SO_2CF_3-PV(b)	C_1-C_2-S-C_3	90
SO_2CF_3-PV(c)	C_1-C_2-S-C_3	90
SO_2CF_3-PE(a)	C_1-C_2-S-C_3	90
SO_2CF_3-PE(b)	C_1-C_2-S-C_3	90
SO_2CF_3-PE(c)	C_1-C_2-S-C_3	90

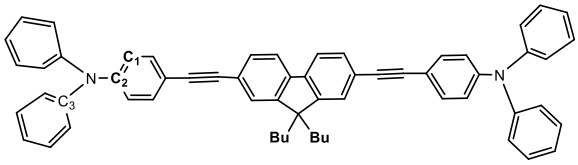
[a]Terminal groups dihedral angles of the studied systems.

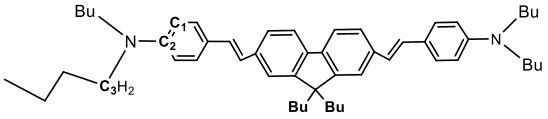


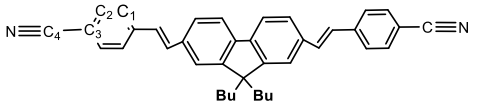


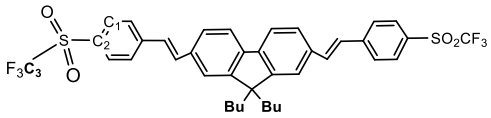


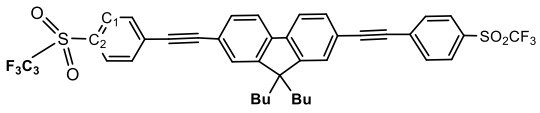












Scheme S1 Atom numbering in the **X-PV** and **X-PE** series of compounds. Hydrogen atoms are omitted for clarity.

Table S2 CAM-B3LYP results (in toluene) of the **X-PV** and **X-PE** series of compounds (S_n is the excited state number, E_{0n} is the transition energy (in eV), λ_{calc} is the wavelength (in nm) and f_{0n} is the oscillator strength)

Compound	S_n	E_{0n}	λ_{calc}	f_{0n}	Main MO transition percentage
OPh-PV					
(a)	1	3.22	385	2.58	HOMO → LUMO (87%)
	2	3.89	319	0.28	HOMO-1 → LUMO (47 %)
	8	4.83	257	0.24	HOMO-2 → LUMO (22 %)
					HOMO-1 → LUMO+1 (19 %)
	17	5.52	225	0.32	HOMO-4 → LUMO (25 %)
(b)	1	3.26	380	2.99	HOMO → LUMO (86%)
	8	4.81	258	0.54	HOMO-2 → LUMO (25 %)
	17	5.52	224	0.32	HOMO-5→ LUMO (33 %)
					HOMO → LUMO+15 (27 %)
	21	5.68	218	0.26	HOMO-8 → LUMO (18 %)
(c)	1	3.25	381	2.62	HOMO → LUMO (87%)
	2	3.90	318	0.24	HOMO-1→ LUMO (48 %)
					HOMO→ LUMO+1 (45 %)
	8	4.83	256	0.25	HOMO-1→ LUMO (22 %)
					HOMO→ LUMO+1 (20 %)
	16	5.68	225	0.20	HOMO → LUMO+11 (24 %)
					HOMO-4 → LUMO (17 %)
(d)	1	3.27	379	3.01	HOMO → LUMO (86%)
	8	4.82	257	0.50	HOMO-2 → LUMO (24 %)
	18	5.54	224	0.24	HOMO → LUMO+15 (20 %)
					HOMO-4 → LUMO (18 %)
					HOMO → LUMO+12 (18 %)
	21	5.68	218	0.25	HOMO → LUMO+2 (15 %)
					HOMO-8 → LUMO (14 %)
OMe-PV					
(a)	1	3.26	381	2.71	HOMO → LUMO (87%)
	8	4.88	254	0.35	HOMO-2 → LUMO (32%)
	15	5.52	225	0.31	HOMO-1 → LUMO+2 (24%)
	28	6.10	203	0.27	HOMO →LUMO+14 (17%)
					HOMO-4 →LUMO+2 (16%)
(b)	1	3.26	380	2.75	HOMO → LUMO (87%)
	8	4.88	254	0.37	HOMO-2 → LUMO (31%)
	16	5.54	224	0.22	HOMO-1→ LUMO+2 (23%)
	28	6.10	203	0.29	HOMO-4 → LUMO+2 (15%)
					HOMO → LUMO+14 (15%)
(c)	1	3.28	378	2.72	HOMO → LUMO (87%)
	8	4.89	254	0.31	HOMO-2 → LUMO (31%)
	16	5.55	224	0.31	HOMO-3 → LUMO (19%)

	26	6.03	206	0.29	HOMO-1 → LUMO+2 (15%) HOMO-2 → LUMO+3 (11%)
(d)	1 8 16 26	3.29 4.89 5.56 6.06	377 253 223 205	2.76 0.34 0.24 0.36	HOMO → LUMO (87%) HOMO-2 → LUMO (30%) HOMO-1 → LUMO+1 (22%) HOMO-1 → LUMO+2 (17%) HOMO-4 → LUMO+2 (8%)
NH_2-PV					
(a)	1 7 18 27	3.20 4.72 5.43 5.88	387 262 227 211	2.84 0.37 0.24 0.15	HOMO → LUMO (85%) HOMO-2 → LUMO (35 %) HOMO-1 → LUMO+1 (24 %) HOMO-1 → LUMO+2 (31 %) HOMO-3 → LUMO (31 %) HOMO → LUMO+10 (31 %)
(b)	1 7 18 28	3.22 4.74 5.42 5.90	386 262 226 210	2.85 0.29 0.30 0.27	HOMO → LUMO (85%) HOMO-2 → LUMO (34 %) HOMO-3 → LUMO (33 %) HOMO-1 → LUMO+2 (23 %) HOMO-2 → LUMO+10 (23 %)
NPh_2-PV					
(a)	1 2 7 28	3.04 3.48 4.27 5.47	408 356 290 227	3.10 0.17 0.57 0.35	HOMO → LUMO (76%) HOMO-1 → LUMO (48%) HOMO → LUMO+1 (38%) HOMO-1 → LUMO+4 (43 %) HOMO-7 → LUMO (24 %) HOMO-8 → LUMO+1 (16 %)
(b)	1 8 18 21	3.05 4.27 4.27 5.47	406 291 290 227	3.14 0.21 0.39 0.39	HOMO → LUMO (79%) HOMO-1 → LUMO+4 (41 %) HOMO-1→ LUMO+5 (42 %) HOMO → LUMO+5 (34 %) HOMO-7→ LUMO (13 %) HOMO-6→ LUMO (10 %)
NPh_2-PE					
(a)	1 7 27 29	3.25 4.33 5.56 5.60	382 287 223 221	3.51 0.56 0.28 0.17	HOMO → LUMO (72%) HOMO-1 → LUMO+6 (44 %) HOMO-4 → LUMO (31 %) HOMO-8 → LUMO (21 %) HOMO-7 → LUMO+1 (17 %)

	1	3.26	380	3.53	HOMO → LUMO (72%)
	7	4.32	287	0.56	HOMO-1 → LUMO+6 (30 %)
					HOMO → LUMO+5 (37 %)
(b)	27	5.58	222	0.34	HOMO-4 → LUMO (34 %)
	29	5.60	221	0.15	HOMO-8 → LUMO (20 %)
					HOMO-8→ LUMO+1 (13 %)
NBu_2-PV					
	1	3.05	407	2.88	HOMO → LUMO (83%)
	2	3.59	345	0.18	HOMO-1 → LUMO (59%)
(a)					HOMO → LUMO+1 (35%)
	19	5.39	230	0.25	HOMO-4 → LUMO (28%)
					HOMO-1 → LUMO+2 (15%)
	29	5.67	217	0.18	HOMO-6 → LUMO (14%)
	1	3.14	404	2.89	HOMO → LUMO (82%)
	7	4.56	272	0.28	HOMO-2 → LUMO (37%)
(b)	19	5.41	229	0.21	HOMO-4 → LUMO (34%)
					HOMO-1 → LUMO+2 (26%)
	27	5.17	217	0.19	HOMO-7 → LUMO (23 %)
CN-PV					
	1	3.16	392	2.95	HOMO → LUMO (86%)
(a)	6	4.72	263	0.24	HOMO-1 → LUMO+1 (27 %)
	9	5.13	242	0.22	HOMO-3→ LUMO (39 %)
	13	5.52	225	0.29	HOMO → LUMO+4 (28 %)
					HOMO-6 → LUMO+1 (15%)
	1	3.17	391	2.97	HOMO → LUMO (86%)
(b)	6	4.23	262	0.20	HOMO-1 → LUMO+1 (26%)
	9	5.17	240	0..25	HOMO-3 → LUMO (37%)
	13	5.53	224	0.26	HOMO → LUMO+4 (25%)
					HOMO-5 → LUMO (20%)
SO_2CF_3-PV					
	1	3.14	395	2.90	HOMO → LUMO (86 %)
	6	4.76	261	0.23	HOMO-1 → LUMO+1 (29%)
(a)					HOMO → LUMO+2 (22%)
	9	5.11	243	0.25	HOMO-3 → LUMO (44%)
	23	6.15	202	0.40	HOMO-1 → LUMO+6 (15%)
	1	3.14	395	2.89	HOMO → LUMO (86 %)
	6	4.75	261	0.23	HOMO-1 → LUMO+1 (29 %)
(b)					HOMO → LUMO+2 (22 %)
	9	5.11	243	0.25	HOMO-3 → LUMO (44 %)
	23	6.15	202	0.42	HOMO-3 → LUMO+5 (15 %)
					HOMO-1 → LUMO+6 (13 %)

(c)	1 6 9 23	3.13 4.75 5.11 6.15	396 261 244 202	2.89 0.23 0.25 0.42	HOMO → LUMO (86%) HOMO-1 → LUMO+1 (29%) HOMO → LUMO+2 (21 %) HOMO-3 → LUMO (12%) HOMO-1 → LUMO+5 (13%) HOMO-1 → LUMO+6 (13%)
SO_2CF_3-PE					
(a)	1 13 29 30	3.35 5.67 6.35 6.39	371 219 195 194	2.89 0.52 0.78 0.42	HOMO → LUMO (84%) HOMO → LUMO+4 (42%) HOMO-3 → LUMO+5 (34%) HOMO-3 → LUMO+5 (17%)
(b)	1 7 13 28	3.35 4.89 5.67 6.35	370 254 219 196	2.88 0.11 0.52 0.97	HOMO → LUMO (84 %) HOMO → LUMO+2 (20%) HOMO→ LUMO+4 (42%) HOMO-3 → LUMO+5 (37%)
(c)	1 7 13 28	3.35 4.88 5.66 6.33	370 254 219 196	2.87 0.18 0.54 1.00	HOMO → LUMO (84 %) HOMO → LUMO+2 (27 %) HOMO → LUMO+4 (26 %) HOMO → LUMO+8 (27 %) HOMO-3 → LUMO+5 (43%)

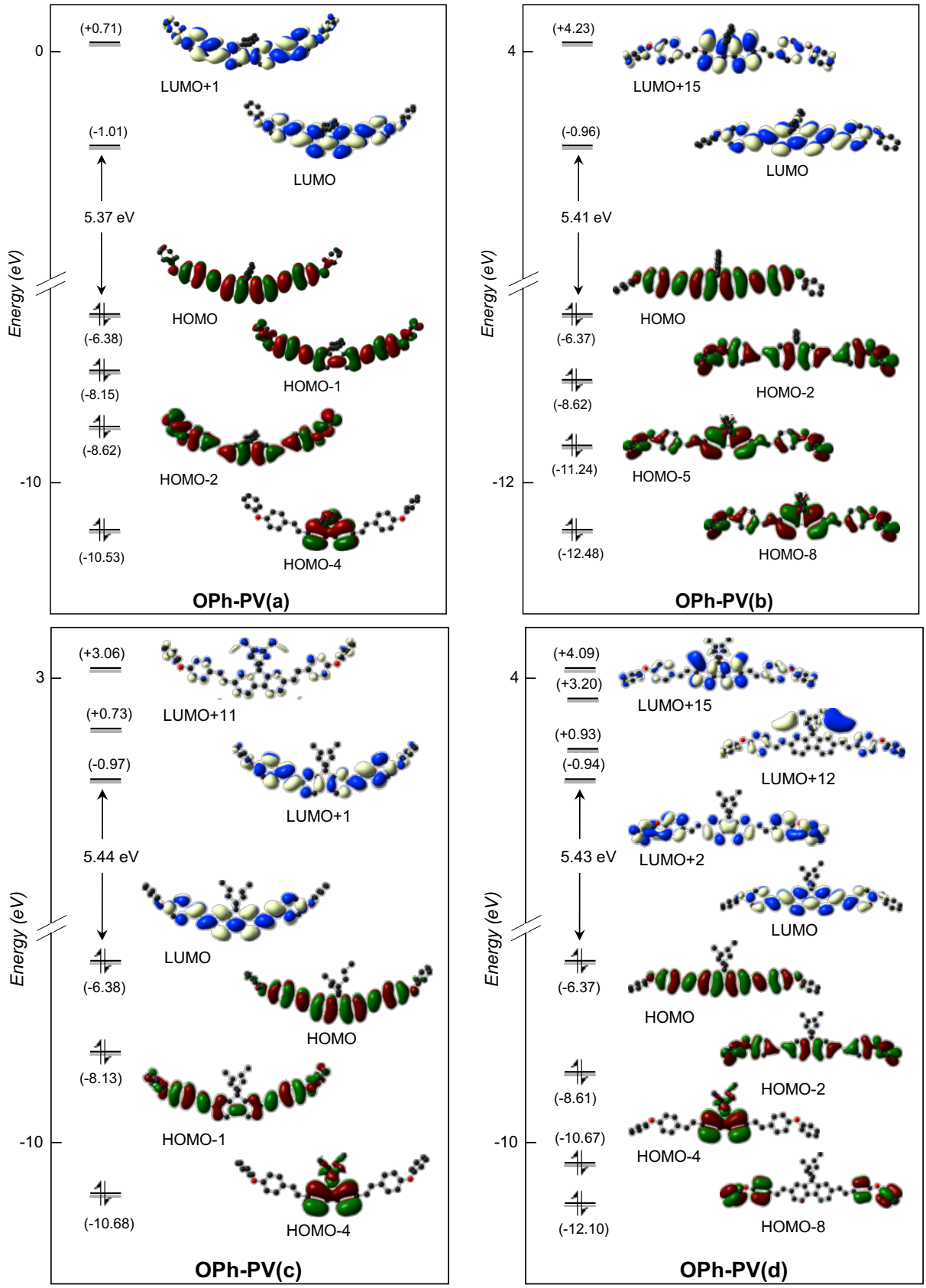


Figure S2 Frontier MO diagrams of **OPh-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

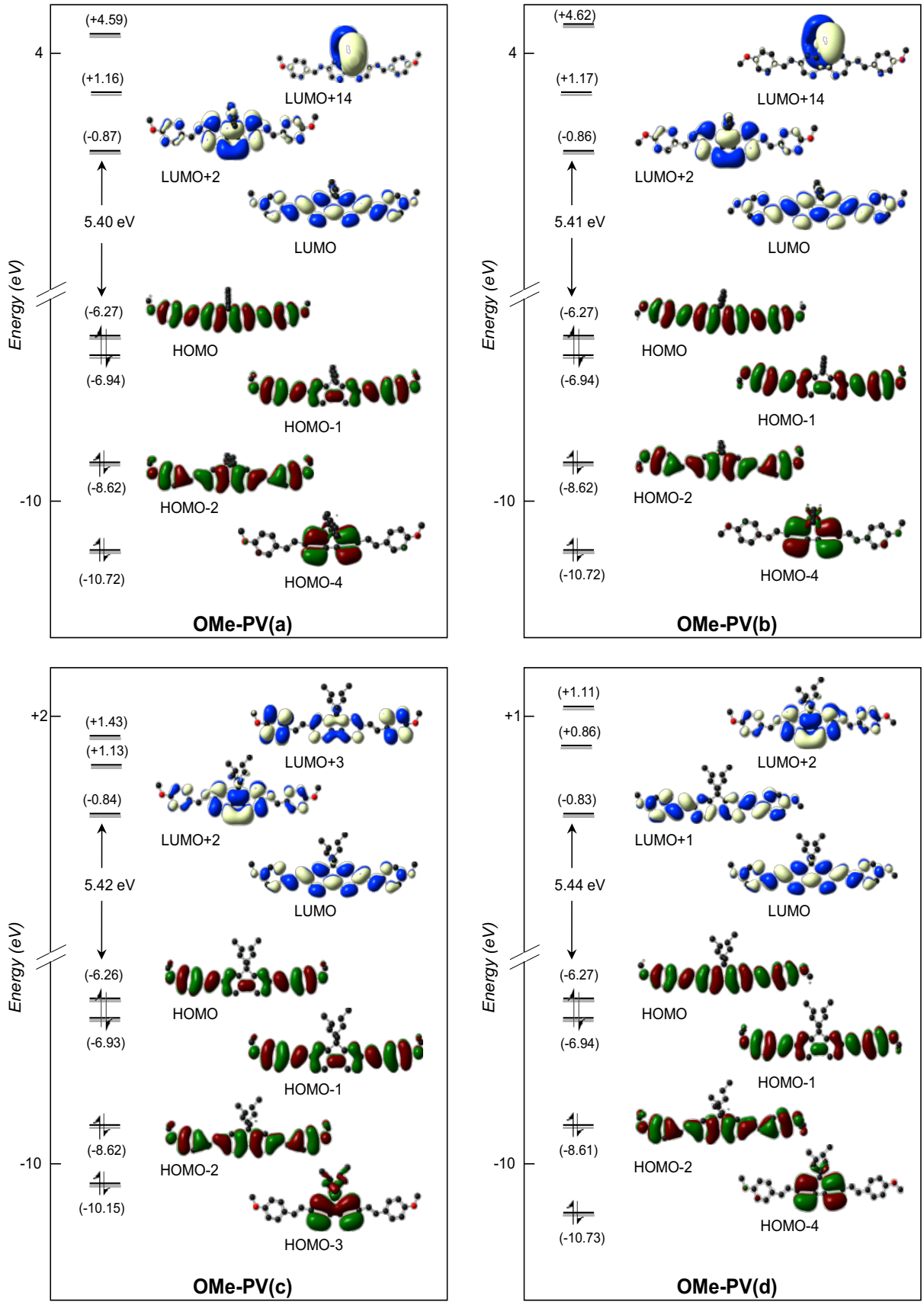


Figure S3 Frontier MO diagrams of **OMe-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

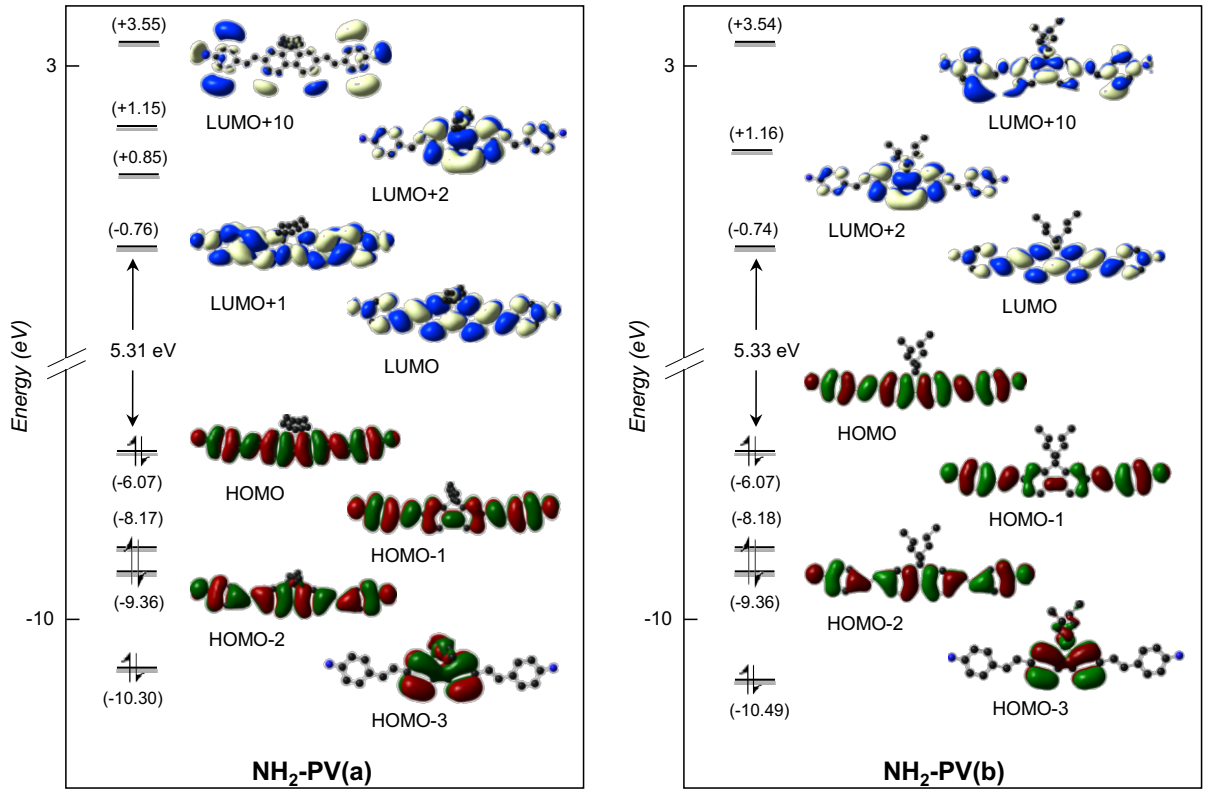


Figure S4 Frontier MO diagrams of **NH_2-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

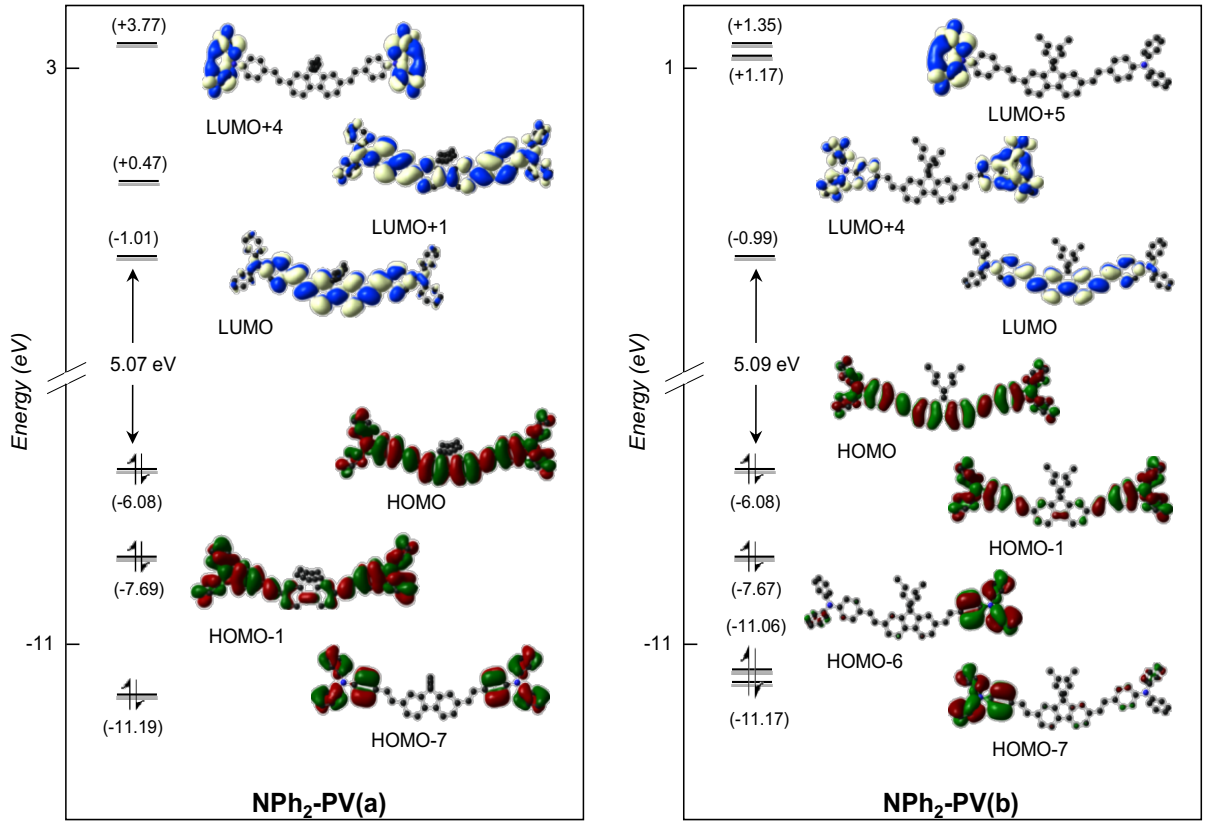


Figure S5 Frontier MO diagrams of **NPh_2-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

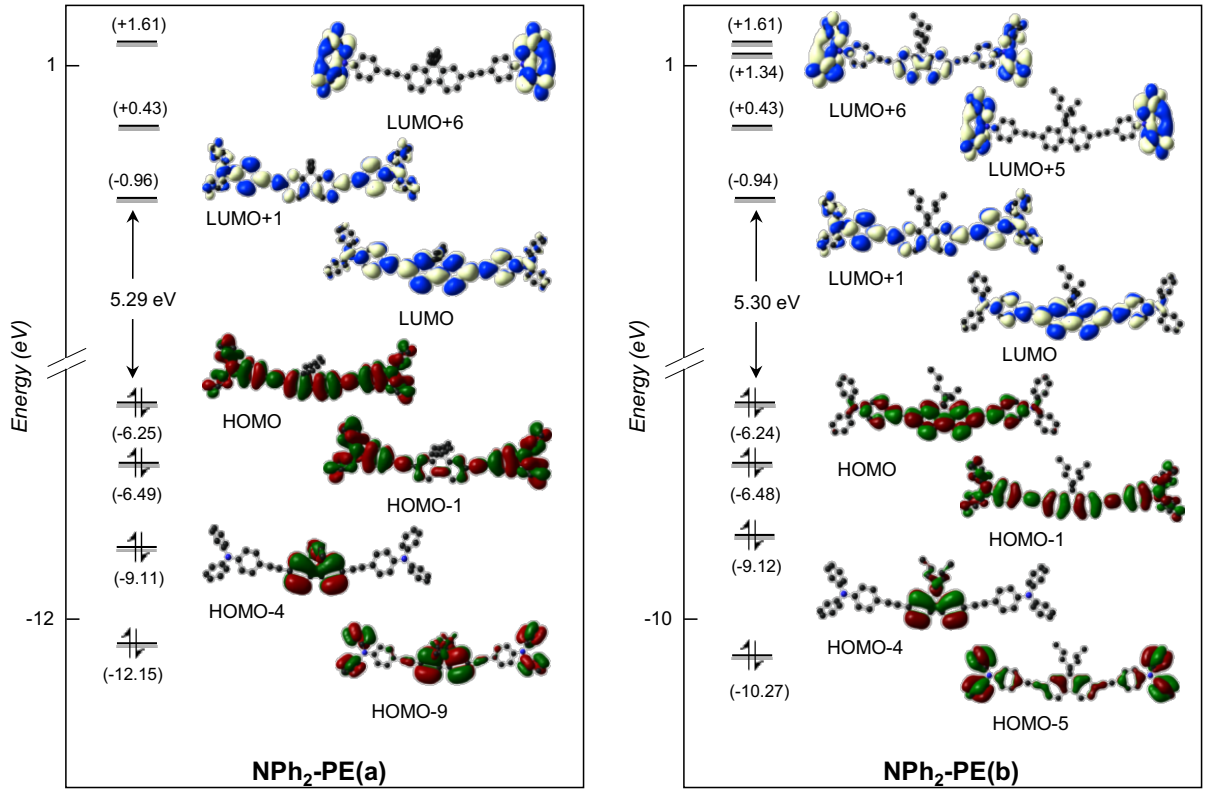


Figure S6 Frontier MO diagrams of **NPh_2-PE** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

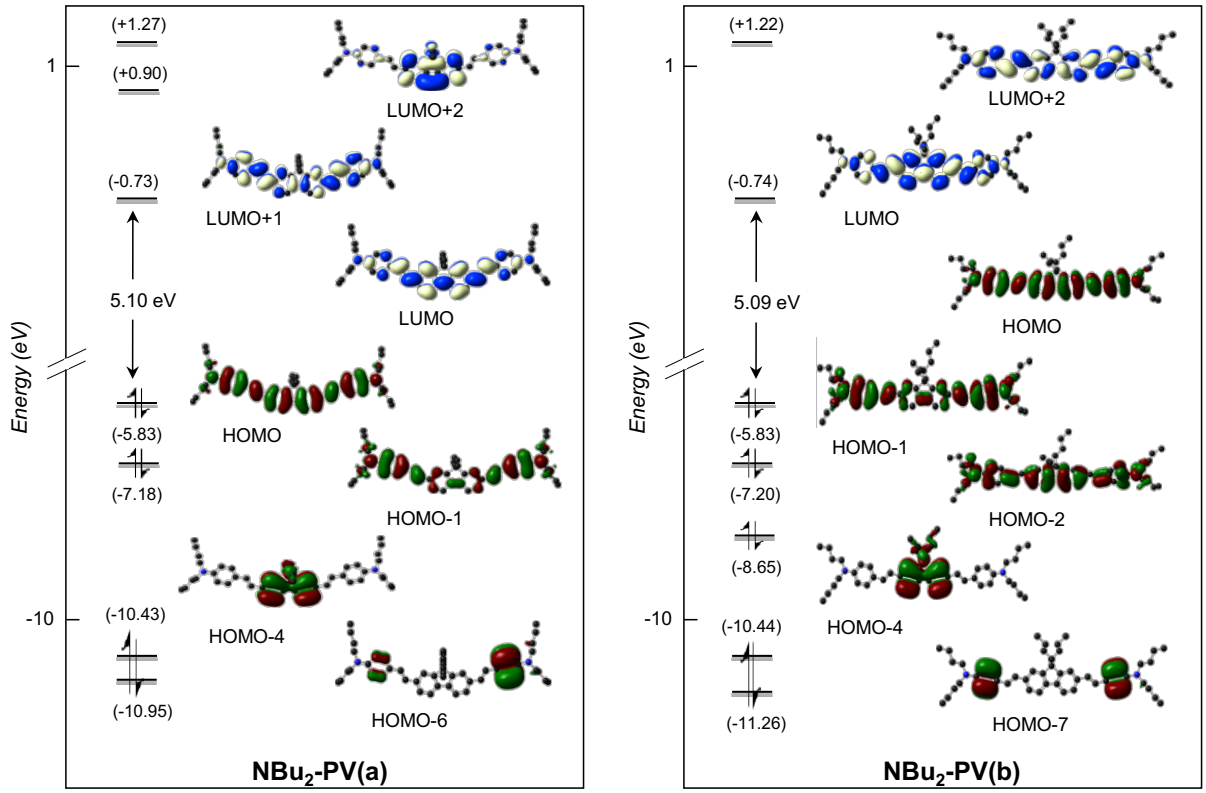


Figure S7 Frontier MO diagram of **NBu_2-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

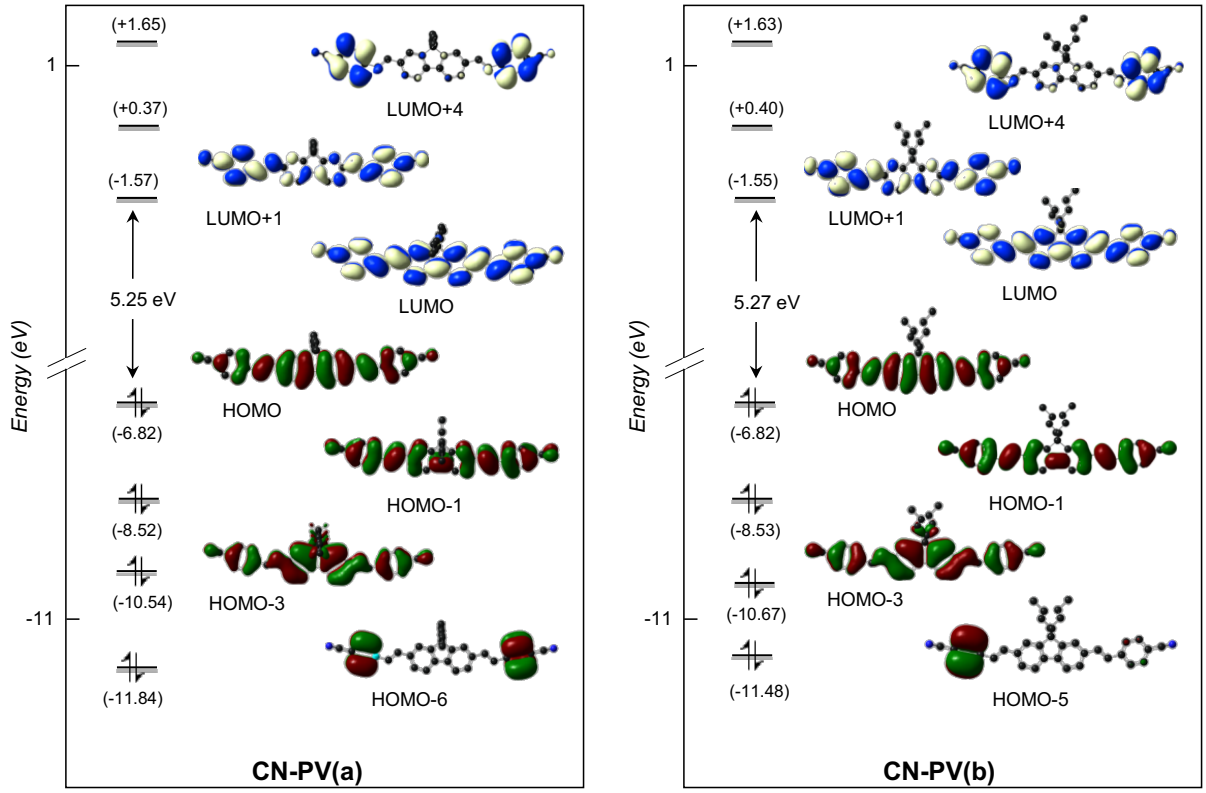


Figure S8 Frontier MO diagrams of **CN-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

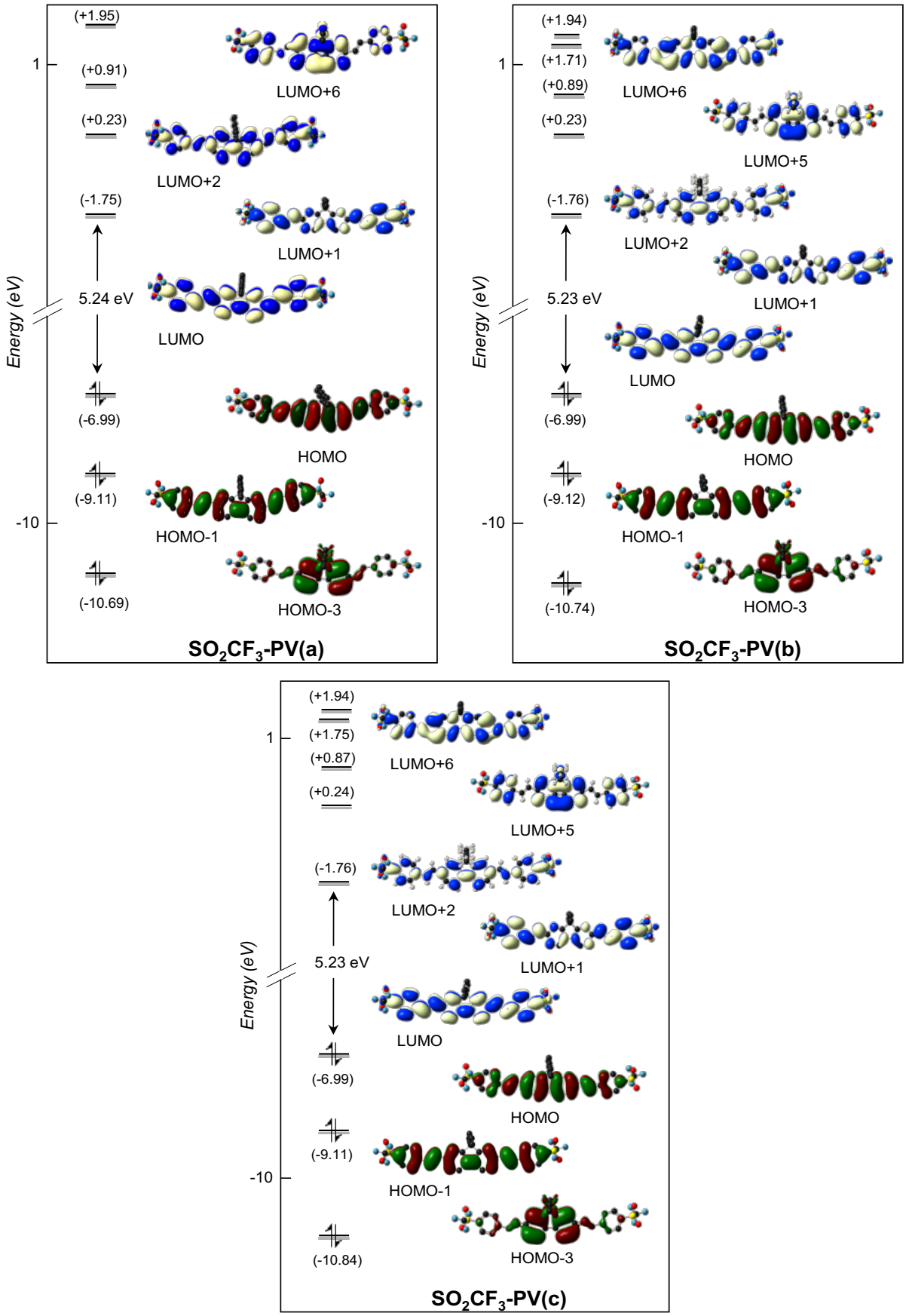


Figure S9 Frontier MO diagrams of **SO_2CF_3-PV** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

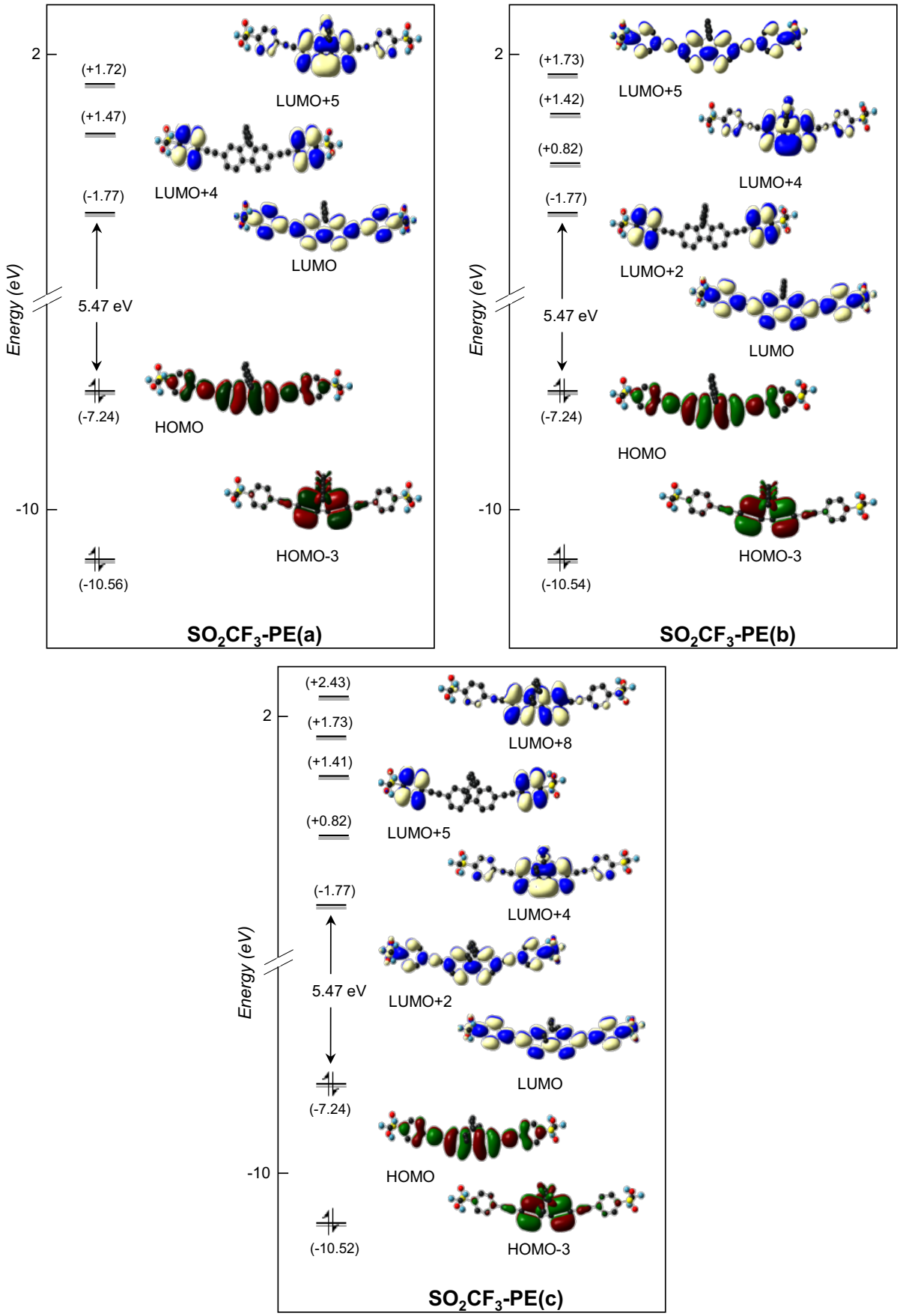


Figure S10 Frontier MO diagrams of **SO_2CF_3-PE** conformers. Contour isodensity values are ± 0.015 $(e/bohr^3)^{1/2}$.

Table S3 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **OPh-PV(*a*)**

S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.59	3.54	3.49	3.38	3.30	3.27	3.24	3.21	2.63	2.46
λ^{OPA}	345	350	355	367	376	379	383	386	471	504
f_{0n}	0.147 10^{-4}	0.311 10^{-1}	0.217	0.267	0.380 10^{-1}	0.214	0.642 10^{-1}	0.628 10^{-1}	0.159 10^{-2}	1.695

Table S4 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **OPh-PV(*a*)** calculated at the SAOP/DZP level of theory

ω^{TPA}	1.76	1.72	1.68	1.64	1.60	1.55	1.46	1.40	1.36	1.32	1.28	1.24	1.18	1,15	1.10	1.05	1.00	0.95
λ^{TPA}	705	720	738	756	775	800	850	885	910	939	968	1000	1051	1080	1127	1180	1240	1305
σ_2	2090	1465	929	943	869	673	998	1990	3923	5266	4010	1542	487	307	159	91	55	34

Table S5 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **OMe-PV(*a*)**

S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.85	3.66	3.60	3.54	3.47	3.45	3.40	3.32	2.65	2.50
λ^{OPA}	322	339	344	350	357	359	365	373	468	496
f_{0n}	0.231 10^{-2}	0.182 10^{-1}	0.624 10^{-1}	0.282 10^{-1}	0.894 10^{-1}	0.285 10^{-1}	0.484	0.991 10^{-1}	0.115 10^{-1}	1.590

Table S6 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **OMe-PV(*a*)** calculated at the SAOP/DZP level of theory

ω^{TPA}	1.76	1.66	1.60	1.55	1.45	1.37	1.33	1.30	1.27	1.24	1.20	1.18	1.10	1,07	1.03	1.00	0.95
λ^{TPA}	705	747	775	800	827	905	932	954	975	1000	1033	1051	1107	1159	1204	1240	1305
σ_2	341	485	402	437	929	3163	5599	3653	2364	916	431	311	107	64	51	33	25

Table S7 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NH_2-PV(*a*)**

S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.70	3.63	3.48	3.44	3.37	3.30	3.27	3.25	2.55	2.43
λ^{OPA}	335	342	356	360	368	376	379	382	486	510
f_{0n}	0.807 10^{-2}	0.164 10^{-5}	0.300 10^{-1}	0.941 10^{-4}	0.135 10^{-1}	0.323	0.677 10^{-2}	0.555	0.528 10^{-4}	1.541

Table S8 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NH_2-PV(*a*)** calculated at the SAOP/DZP level of theory

ω^{TPA}	1.76	1.74	1.68	1.64	1.55	1.47	1.40	1.38	1.33	1.30	1.28	1.24	1,21	1.18	1.10	0.99	0.95
λ^{TPA}	705	713	738	756	800	844	886	900	932	954	969	1000	1025	1051	1127	1250	1305
σ_2	286	285	341	408	734	544	998	1273	2815	4776	6813	3056	1474	772	207	57	24

Table S9 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NPh_2-PV(*a*)**

S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.14	3.07	3.06	2.95	2.94	2.85	2.75	2.71	2.17	2.06
λ^{OPA}	395	404	405	420	422	435	451	458	571	602
f_{0n}	0.542 10^{-2}	0.216 10^{-1}	0.117 10^{-2}	0.500 10^{-2}	0.675 10^{-2}	0.359 10^{-1}	1.148	0.485 10^{-1}	0.677 10^{-2}	1.476

Table S10 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NPh_2-PV(a)** calculated at the SAOP/DZP level of theory

ω^{TPA}	1.76	1.72	1.675	1.64	1.57	1.47	1.42	1.36	1.31	1.24	1.18	1.13	1.10	1.06	1.03	0.99	0.95
λ^{TPA}	705	721	740	756	790	844	873	912	947	1000	1050	1097	1127	1170	1204	1250	1305
σ_2	2645	7557	3318	2024	1394	1214	1333	1351	1285	1485	3680	8209	12401	8185	3902	1574	745

Table S11 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NPh_2-PE(*a*)**

S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.23	3.13	3.12	3.02	3.01	3.00	2.95	2.93	2.35	2.23
λ^{OPA}	384	396	397	411	412	413	420	423	528	556
f_{0n}	0.318 10^{-2}	0.197 10^{-1}	0.620 10^{-3}	0.486 10^{-1}	0.217 10^{-2}	0.170 10^{-3}	1.393	0.259 10^{-1}	0.417 10^{-2}	1.563

Table S12 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NPh_2-PE(*a*)** calculated at the SAOP/DZP level of theory

ω^{TPA}	1.76	1.72	1.675	1.62	1.58	1.50	1.46	1.37	1.31	1.27	1.24	1.18	1,12	1.07	1.03	1.00	0.95
λ^{TPA}	705	720	740	765	785	827	850	900	950	975	1000	1051	1107	1159	1204	1240	1305
σ_2	3640	2303	1768	1392	1394	1834	2062	1673	2439	3788	5933	13710	4528	1493	734	467	264

Table S13 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **CN-PV(*a*)**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.65	3.56	3.55	3.45	3.42	3.34	3.30	3.26	2.53	2.38
λ^{OPA}	340	348	349	359	363	371	376	380	490	521
f_{0n}	0.130 10^{-1}	0.108 10^{-1}	0.426 10^{-2}	0.208	0.281	0.595 10^{-1}	0.723 10^{-3}	0.420	0.766 10^{-2}	1.646

Table S14 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **CN-PV(*a*)** calculated at the SAOP/DZP level of theory																	
ω^{TPA}	1.76	1.65	1.60	1.55	1.45	1.37	1.33	1.30	1.27	1.24	1.20	1.18	1.10	1,07	1.03	1.00	0.95
λ^{TPA}	705	747	765	800	855	905	932	954	975	1000	1033	1051	1127	1159	1204	1240	1305
σ_2	467	354	365	385	635	1652	2493	4305	6220	4566	1958	1134	279	198	114	81	49

Table S15 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NBu_2-PV(*a*)**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.94	3.90	3.87	3.85	3.49	3.18	3.12	2.75	2.12	2.07
λ^{OPA}	315	318	320	322	355	390	397	451	585	599
f_{0n}	0.165 10^{-2}	0.259 10^{-2}	0.384 10^{-2}	0.181 10^{-1}	0.698 10^{-1}	0.369	0.142 10^{-1}	0.789	0.678 10^{-2}	1.6

Table S16 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NBu_2-PV(*a*)** calculated at the SAOP/DZP level of theory														
ω^{TPA}	1.76	1.66	1.61	1.50	1.45	1.36	1.30	1.25	1.20	1.15	1.08	1.03	1.00	0.95
λ^{TPA}	705	747	770	827	855	912	954	992	1033	1078	1150	1204	1240	1305
σ_2	1260	685	623	965	862	1135	1692	958	1265	3156	14520	6584	2654	265

Table S17 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **SO_2CF_3-PV(*a*)**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.59	3.57	3.56	3.53	3.39	3.34	3.28	3.23	2.54	2.37
λ^{OPA}	345	347	348	351	366	371	378	384	488	523
f_{0n}	0.448 10^{-1}	0.359 10^{-1}	0.749 10^{-3}	0.178	0.418	0.802 10^{-1}	0.194	0.144 10^{-1}	0.715 10^{-2}	1.678

Table S18 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **SO_2CF_3-PV(*a*)** calculated at the SAOP/DZP level of theory																	
ω^{TPA}	1.76	1.67	1.61	1.55	1.50	1.45	1.40	1.35	1.30	1.27	1.24	1.18	1.20	1,10	1.03	1.00	0.95
λ^{TPA}	705	743	770	800	827	855	886	920	954	976	1000	1051	1033	1127	1204	1240	1305
σ_2	518	413	380	415	508	692	1075	2053	4954	6523	4468	1063	1640	270	152	80	48

Table S19 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n}calculated at the SAOP/DZP level of theory of molecule **SO_2CF_3-PE(*a*)**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.68	3.64	3.63	3.62	3.53	3.45	3.44	3.36	2.73	2.53
λ^{OPA}	337	341	342	443	351	359	360	369	454	490
f_{0n}	0.345 10^{-1}	0.166 10^{-1}	0.857 10^{-3}	0.322 10^{-1}	0.714	0.359 10^{-1}	1.161	0.590 10^{-2}	0.260 10^{-2}	1.708

Table S20 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **SO_2CF_3-PE(*a*)** calculated at the SAOP/DZP level of theory																	
ω^{TPA}	1.76	1.68	1.60	1.55	1.50	1.44	1.40	1.37	1.33	1.30	1.25	1.18	1.12	1,10	1.03	1.00	0.95
λ^{TPA}	705	738	775	800	827	860	885	905	930	955	990	1051	1107	1127	1204	1240	1305
σ_2	376	419	501	575	850	1925	3283	7615	3565	2156	643	320	126	101	80	55	26

Table S21 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NH_2-PE**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.80	3.71	3.65	3.55	3.54	3.47	3.46	3.37	2.79	2.61
λ^{OPA}	326	334	340	349	350	357	358	368	444	475
f_{0n}	0.243 10^{-2}	0.494 10^{-2}	0.218	0.590	0.205 10^{-1}	0.702 10^{-4}	0.468 10^{-2}	0.264 10^{-2}	0.134 10^{-2}	1.645

Table S22 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NH_2-PE** calculated at the SAOP/DZP level of theory												
ω^{TPA}	1.76	1.65	1.60	1.50	1.45	1.40	1.35	1.30	1,20	1.10	1.00	0.95
λ^{TPA}	705	752	775	827	855	886	919	954	1033	1127	1240	1305
σ_2	256	356	557	1394	3092	7483	5234	899	187	63	26	24

Table S23 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **CN-PE**							
S_n	7	6	5	4	3	2	1
ω^{OPA}	3.58	3.53	3.47	3.44	3.43	2.73	2.56
λ^{OPA}	346	351	357	361	362	454	485
f_{0n}	0.118	0.328	0.347	0.497	0.93810^{-2}	$0.143\ 10^{-2}$	1.702

Table S24 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **CN-PE** calculated at the SAOP/DZP level of theory											
ω^{TPA}	1.76	1.60	1.50	1.45	1.40	1.375	1.35	1.30	1,20	1.00	0.95
λ^{TPA}	705	775	827	855	886	902	919	954	1033	1240	1305
σ_2	264	549	1159	2201	5315	7192	6007	1898	312	37	16

Table S25 Theoretical results of OPA wavelengths (nm), OPA energies (eV) and f_{0n} calculated at the SAOP/DZP level of theory of molecule **NBu_2-PV-SO_2CF_3**										
S_n	10	9	8	7	6	5	4	3	2	1
ω^{OPA}	3.43	3.39	3.21	3.19	3.15	3.08	2.80	2.67	2.55	1.61
λ^{OPA}	362	366	386	389	394	403	443	464	486	770
f_{0n}	$0.423\ 10^{-2}$	$0.570\ 10^{-1}$	$0.137\ 10^{-2}$	$0.154\ 10^{-1}$	$0.249\ 10^{-1}$	0.387	$0.110\ 10^{-1}$	0.302	1.224	0.471

Table S26 TPA wavelengths (nm), TPA energies (eV) and σ_2 (GM) associated with the different states of molecule **NBu_2-PV-SO_2CF_3** calculated at the SAOP/DZP level of theory													
ω^{TPA}	1.55	1.50	1.45	1.40	1.34	1.32	1.30	1.28	1.24	1,20	1.10	1.00	0.95
λ^{TPA}	800	827	855	886	925	940	954	969	1000	1033	1127	1240	1305
σ_2	1236	1364	1564	1984	2706	2972	3290	3322	1864	942	553	691	1534

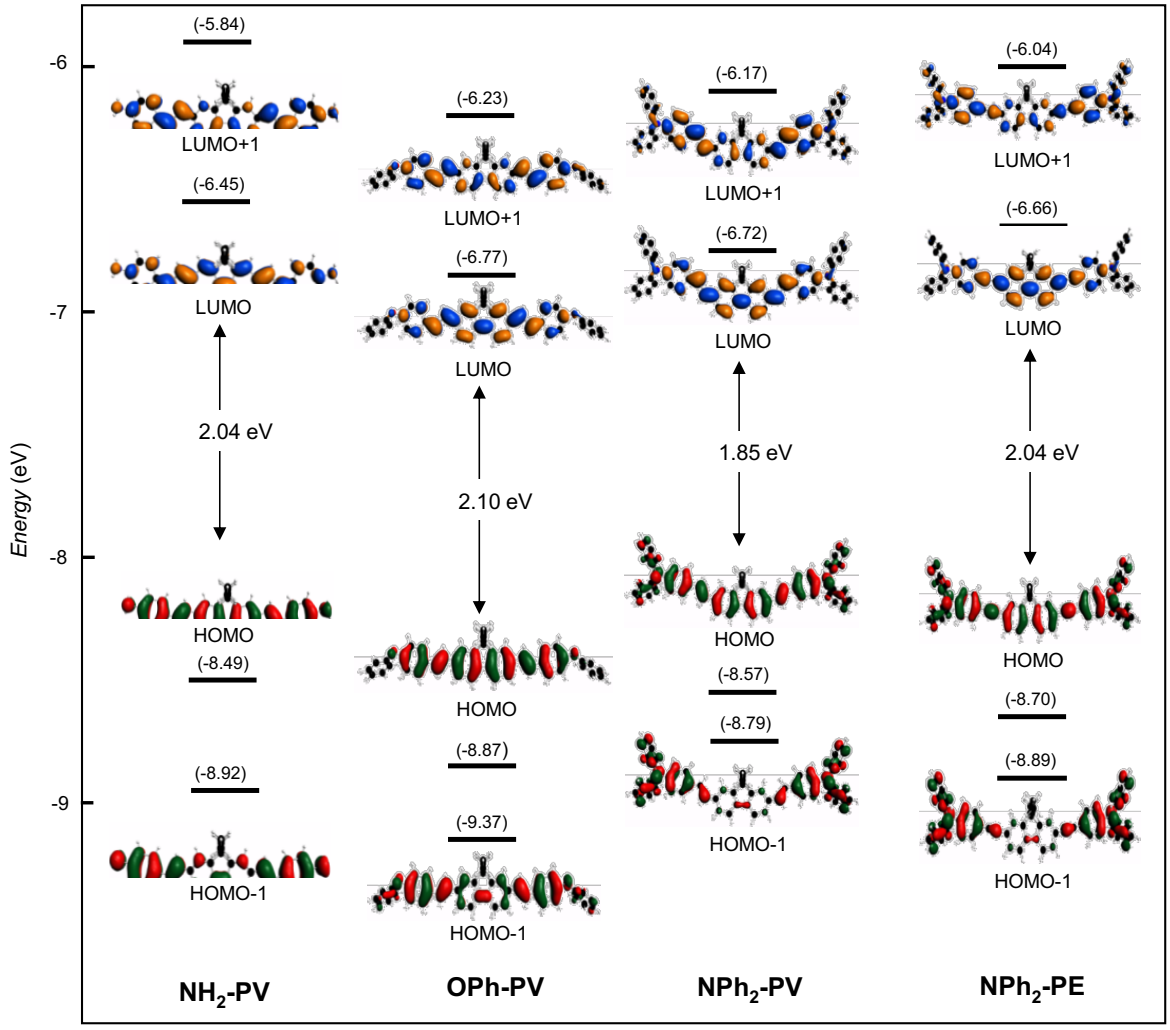


Figure S11 SAOP/DZP frontier MO diagrams of **OPh-PV**, **NH_2-PV**, **NPh_2-PV**, and **NPh_2-PE** in their most stable conformer form (***a***). Contour isodensity values: ±0.015 $(e/bohr^3)^{1/2}$.

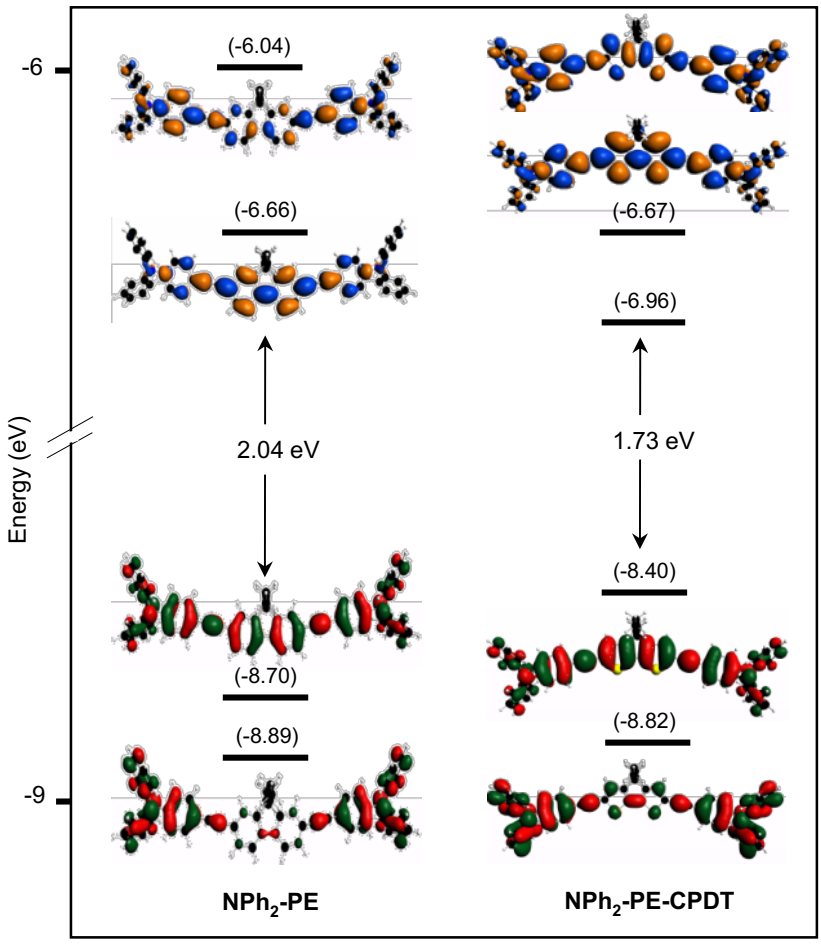


Figure S12 SAOP/DZP frontier MO diagrams of **NPh_2-PE** (conformer ***a***, left) and **NPh_2-PE-CPDT** (right). Contour isodensity values: ±0.015 $(e/bohr^3)^{1/2}$.

Cartesian coordinates of optimized molecules

1. Molecule **OPh-PV** (PBE0/6-31+G(d)/toluene)

OPh-PV(*a*)				**OPh-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	-9.311960	-1.158300	-0.348424	C	-9.67410400	-0.50066200	-1.18889500
C	-7.953204	-1.403106	-0.474307	C	-8.31065000	-0.42997900	-1.45289900
C	-6.997101	-0.496404	0.018615	C	-7.35222800	-0.39925200	-0.42667700
C	-7.476503	0.662883	0.650077	C	-7.82490200	-0.44767400	0.89740100
C	-8.835945	0.920384	0.789564	C	-9.18120700	-0.51261100	1.17744500
C	-9.757051	0.006143	0.281268	C	-10.10978400	-0.53535500	0.13460100
H	-10.045069	-1.861854	-0.732840	H	-10.39066400	-0.53181600	-2.00428500
H	-7.635914	-2.315850	-0.970880	H	-7.97751200	-0.40481300	-2.48857600
H	-6.763299	1.380498	1.050811	H	-7.12525500	-0.43068000	1.72839300
H	-9.175589	1.821461	1.291496	H	-9.53984300	-0.54826300	2.20231800
C	-5.554142	-0.696165	-0.088434	C	-5.93825500	-0.32216100	-0.78478000
C	-4.919482	-1.744811	-0.652007	C	-4.88851100	-0.26924700	0.06089000
C	-3.476940	-1.945020	-0.759849	C	-3.47383700	-0.19192900	-0.29398900
C	-1.175347	-1.288214	-0.405460	C	-1.17214600	-0.06509300	0.46106100
C	-0.729590	-2.463244	-1.042085	C	-0.72828100	-0.04050200	-0.87183200
C	0.000216	-0.439647	0.053073	C	0.00000400	0.00000400	1.42642700
C	1.175322	-1.287836	-0.407339	C	1.17215700	0.06509500	0.46106300
C	0.728934	-2.462968	-1.043324	C	0.72829400	0.04049400	-0.87183100
C	3.476563	-1.943812	-0.765542	C	3.47384900	0.19192500	-0.29398300
C	4.919213	-1.743278	-0.659721	C	4.88852200	0.26924600	0.06089700
C	5.554387	-0.695989	-0.094199	C	5.93826900	0.32214600	-0.78477100
C	6.997444	-0.495917	0.010877	C	7.35224000	0.39923700	-0.42666500
C	7.953025	-1.399500	-0.488780	C	8.31066500	0.42996300	-1.45288600
C	9.311889	-1.154828	-0.364099	C	9.67411800	0.50064600	-1.18887900
C	9.757712	0.006393	0.271066	C	10.10979600	0.53534100	0.13461700
C	8.837168	0.917587	0.785811	C	9.18121700	0.51259700	1.17746000
H	9.177297	1.816165	1.291859	H	9.53985100	0.54824900	2.20233300
C	7.477560	0.660231	0.647480	C	7.82491200	0.44766000	0.89741300
H	10.044572	-1.855951	-0.753739	H	10.39067900	0.53179900	-2.00426800
H	7.635158	-2.309592	-0.989829	H	7.97752800	0.40479500	-2.48856300
H	6.764824	1.375437	1.053325	H	7.12526400	0.43066500	1.72840400
C	0.001392	-0.242658	1.586644	C	0.06983500	-1.25277300	2.33021800
C	0.002416	-1.517236	2.424198	C	0.14223500	-2.59444100	1.60855600
H	-0.877403	0.364427	1.849930	H	-0.80987200	-1.24220600	2.99056600
H	0.880285	0.364897	1.848511	H	0.94515200	-1.14604900	2.98784600
C	0.003637	-1.232366	3.923986	C	0.20960800	-3.77542000	2.57361100
H	-0.877316	-2.125578	2.172305	H	-0.73377600	-2.71055100	0.95540200
C	0.004734	-2.501460	4.768706	C	0.28210800	-5.12084500	1.86033500
1	0.882622	-0.622085	4.177759	H	1.08499000	-3.66014500	3.22925300
H	-0.875248	-0.622583	4.179291	H	-0.67008000	-3.75694800	3.23333900
H	0.005603	-2.271164	5.840417	H	0.32948500	-5.95206100	2.57339500
H	-0.880085	-3.115469	4.559854	H	-0.59683300	-5.27755200	1.22280000
H	0.889536	-3.114966	4.558308	H	1.17005000	-5.18022700	1.21878000
C	-0.000523	0.952374	-0.619976	C	-0.06983100	1.25278300	2.33021400
C	-0.001681	0.957515	-2.145109	C	-0.14227700	2.59444600	1.60854700
C	-0.002357	2.369396	-2.725703	C	-0.20967200	3.77542800	2.57359900

C	-0.003494	2.383934	-4.250160	C	-0.28221200	5.12084800	1.86031800
H	-0.881086	2.915636	-2.352984	H	-1.08504400	3.66013200	3.22924900
H	0.876738	2.915935	-2.354292	H	0.67002300	3.75698000	3.23331900
H	-0.003966	3.407456	-4.642633	H	-0.32960400	5.95206500	2.57337500
H	0.881086	1.873226	-4.650449	H	0.59671900	5.27757400	1.22277400
H	-0.888484	1.872911	-4.649138	H	-1.17016100	5.18020500	1.21877100
H	0.882020	-2.125133	2.170797	H	1.02266800	-2.61367500	0.95130200
H	0.877723	0.413779	-2.517229	H	0.73372300	2.71057700	0.95538300
H	-0.881464	0.413478	-2.515895	H	-1.02271900	2.61365300	0.95130300
H	0.878494	1.504300	-0.255439	H	0.80988900	1.24223800	2.99054400
H	-0.879151	1.504032	-0.254098	H	-0.94513200	1.14604400	2.98786000
C	-2.525450	-1.029291	-0.264275	C	-2.52486200	-0.13970600	0.74643200
H	-2.852845	-0.117346	0.230383	H	-2.87250600	-0.15855700	1.77891000
C	2.525565	-1.028431	-0.268385	C	2.52487200	0.13971100	0.74643600
H	2.853442	-0.116282	0.225574	H	2.87251300	0.15856900	1.77891500
C	-11.683950	1.397391	0.450817	C	3.00782100	0.16669600	-1.62448900
C	-11.353769	2.375487	-0.487334	C	1.65305200	0.09201800	-1.91829300
C	-12.678379	1.624316	1.398819	C	-1.65303700	-0.09203300	-1.91829600
C	-12.023502	3.596500	-0.459211	C	-3.00780700	-0.16671000	-1.62449400
H	-10.585450	2.179590	-1.229924	H	-3.71816200	-0.20652000	-2.44559700
C	-13.345980	2.847459	1.411309	H	-1.32455500	-0.07465000	-2.95508300
H	-12.918524	0.840543	2.111574	H	1.32457200	0.07462700	-2.95508100
C	-13.019458	3.838968	0.487192	H	3.71817800	0.20650000	-2.44559100
H	-11.768783	4.359717	-1.190257	H	5.75048600	0.30609300	-1.85809700
H	-14.122467	3.024678	2.151074	H	5.07855100	0.28274700	1.13412800
H	-13.539418	4.792935	0.501127	H	-5.07854200	-0.28273500	1.13412000
C	11.683949	1.397469	0.448995	H	-5.75047100	-0.30612100	-1.85810600
C	12.676635	1.618119	1.400252	O	-11.42794700	-0.66967600	0.48844500
C	11.354495	2.382164	-0.482471	O	11.42795800	0.66965900	0.48846400
C	13.343298	2.841655	1.422819	C	-12.41581400	-0.11372700	-0.29288400
H	12.916232	0.829303	2.107600	C	-13.55778800	-0.88046100	-0.51049100
C	12.023238	3.603440	-0.444315	C	-12.32878300	1.19212600	-0.77562200
H	10.587494	2.191055	-1.227676	C	-14.62280000	-0.33504100	-1.22468800
C	13.017504	3.839647	0.505469	H	-13.59917100	-1.89171000	-0.11593100
H	14.118474	3.014026	2.165099	C	-13.39753400	1.72271700	-1.49434200
H	11.769143	4.371830	-1.170138	H	-11.43741000	1.78367500	-0.58689900
H	13.536740	4.793863	0.527235	C	-14.54639000	0.96489500	-1.72274300
C	3.009846	-3.112725	-1.397899	H	-15.51427200	-0.93345100	-1.39428200
C	1.652720	-3.380771	-1.541366	H	-13.33235100	2.74067600	-1.87024600
C	-1.653869	-3.381534	-1.538304	H	-15.37704500	1.38664600	-2.28196600
C	-3.010852	-3.113969	-1.392601	C	12.41582600	0.11373000	-0.29287700
H	3.737245	-3.824115	-1.783953	C	13.55779600	0.88047200	-0.51047300
H	1.327722	-4.293652	-2.035246	C	12.32879900	-1.19211400	-0.77563800
H	-1.329363	-4.294460	-2.032421	C	14.62280900	0.33506900	-1.22468200
H	-3.738629	-3.825739	-1.777236	H	13.59917500	1.89171400	-0.11589500
O	11.114308	0.144361	0.416077	C	13.39755100	-1.72268900	-1.49437000
O	-11.113419	0.144509	0.428407	H	11.43742800	-1.78367000	-0.58692400
H	4.959599	0.106148	0.342282	C	14.54640200	-0.96485800	-1.72276000
H	5.514985	-2.545556	-1.094720	H	15.51427800	0.93348600	-1.39426700
H	-5.515653	-2.548466	-1.083900	H	13.33237000	-2.74064100	-1.87029300
H	-4.958939	0.107696	0.344290	H	15.37705900	-1.38659600	-2.28199200
OPh-PV(*c*)				**OPh-PV(*d*)**			

atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	8.851894	-0.888499	-0.417900	C	9.670450	-1.550930	-0.433026
C	7.495032	-0.604350	-0.308477	C	8.302614	-1.799776	-0.409975
C	6.985379	0.689560	-0.504750	C	7.355046	-0.763116	-0.432403
C	7.906015	1.701754	-0.831270	C	7.843507	0.554814	-0.488278
C	9.262630	1.436095	-0.937759	C	9.204531	0.819711	-0.505922
C	9.739715	0.140735	-0.726580	C	10.121574	-0.232756	-0.473414
H	9.214973	-1.900927	-0.268111	H	10.379080	-2.373805	-0.422530
H	6.807667	-1.412989	-0.067749	H	7.957369	-2.831345	-0.378993
H	7.561494	2.716916	-1.007642	H	7.152662	1.392861	-0.516446
H	9.968574	2.222297	-1.190235	H	9.575416	1.839988	-0.547802
C	5.548240	0.911314	-0.366249	C	5.935383	-1.105484	-0.398446
C	4.900460	2.093076	-0.427731	C	4.894052	-0.248720	-0.360388
C	3.462737	2.313704	-0.295307	C	3.474203	-0.590123	-0.321909
C	1.175260	1.539347	-0.075103	C	1.176845	0.193752	-0.183383
C	0.726202	2.875127	-0.047548	C	0.725928	-1.137751	-0.202937
C	0.000065	0.567818	0.000271	C	0.006879	1.164114	-0.047715
C	-1.175232	1.539251	0.075278	C	-1.168300	0.192252	0.008712
C	-0.726315	2.875068	0.047231	C	-0.725085	-1.138619	-0.085726
C	-3.462788	2.313456	0.295199	C	-3.469365	-0.588101	0.096782
C	-4.900491	2.092723	0.427669	C	-4.885930	-0.242848	0.186468
C	-5.548160	0.910893	0.366337	C	-5.929407	-1.095876	0.244359
C	-6.985276	0.689014	0.504892	C	-7.345185	-0.748073	0.336555
C	-7.494787	-0.605000	0.308867	C	-8.295715	-1.781365	0.376627
C	-8.851607	-0.889268	0.418400	C	-9.660175	-1.527442	0.463058
C	-9.739531	0.139927	0.726918	C	-10.105125	-0.207256	0.504677
C	-9.262600	1.435373	0.937825	C	-9.184646	0.842382	0.472678
H	-9.968622	2.221547	1.190168	H	-9.550327	1.864573	0.513554
C	-7.906008	1.701168	0.831241	C	-7.827098	0.572403	0.391878
H	-9.214603	-1.901759	0.268817	H	-10.370416	-2.348072	0.501155
H	-6.807333	-1.413601	0.068266	H	-7.955334	-2.814556	0.346373
H	-7.561598	2.716409	1.007373	H	-7.133852	1.408582	0.367387
C	2.524306	1.263733	-0.220971	C	2.538026	0.458475	-0.224115
H	2.866105	0.235788	-0.298954	H	2.908457	1.479741	-0.167021
C	-2.524249	1.263553	0.221256	C	-2.527696	0.459973	0.078042
H	-2.865945	0.235605	0.299655	H	-2.892333	1.484406	0.109875
C	-2.990499	3.638619	0.247574	C	-2.997546	-1.913914	0.024239
C	-1.636125	3.928052	0.130624	C	-1.642029	-2.192876	-0.073156
C	1.635906	3.928173	-0.131316	C	1.636874	-2.192392	-0.304138
C	2.990310	3.638835	-0.248150	C	2.994411	-1.914134	-0.370336
H	3.708068	4.454289	-0.312118	H	3.694614	-2.740667	-0.453403
H	1.298693	4.962011	-0.114501	H	1.293674	-3.224274	-0.325889
H	-1.299016	4.961917	0.113432	H	-1.305122	-3.224539	-0.145354
H	-3.708342	4.454020	0.311253	H	-3.702652	-2.740440	0.032438
H	-4.971283	0.004229	0.184351	H	-5.734300	-2.167800	0.223375
H	-5.481731	3.002582	0.577110	H	-5.083046	0.828943	0.210090
H	5.481624	3.002966	-0.577277	H	5.096334	0.822301	-0.347218
H	4.971453	0.004616	-0.184149	H	5.735353	-2.176696	-0.397133
C	0.005939	-0.286553	1.293376	C	-0.173979	2.070291	-1.292162
C	1.107600	-1.330610	1.447614	C	0.893616	3.127000	-1.559141
H	-0.966788	-0.792577	1.364279	H	-1.147225	2.572229	-1.201552
H	0.044569	0.402974	2.147964	H	-0.257698	1.416116	-2.171006
C	0.933815	-2.163435	2.716458	C	0.542587	4.004861	-2.759064

H	1.122476	-2.005343	0.579564	H	1.027762	3.769350	-0.676962
H	2.088938	-0.839862	1.481261	H	1.861887	2.645328	-1.746766
C	2.036286	-3.199427	2.903321	C	1.603786	5.058176	-3.055864
H	0.907207	-1.493441	3.587498	H	0.399161	3.367799	-3.643352
H	-0.043341	-2.666796	2.688943	H	-0.423763	4.497144	-2.577791
H	1.886603	-3.784320	3.818078	H	1.326647	5.675216	-3.918269
H	2.067156	-3.901530	2.060607	H	1.746981	5.728512	-2.199035
H	3.021137	-2.720815	2.972124	H	2.572196	4.592611	-3.277419
C	-0.005731	-0.287000	-1.292545	C	0.192704	1.966159	1.265425
C	-1.107276	-1.331231	-1.446398	C	-0.871589	3.000186	1.619980
H	0.967051	-0.792941	-1.363285	H	1.166898	2.471751	1.212796
H	-0.044445	0.402232	-2.147368	H	0.277237	1.243052	2.088376
C	-0.933469	-2.164434	-2.714992	C	-0.511649	3.782794	2.881639
H	-1.122016	-2.005695	-0.578136	H	-1.010844	3.708654	0.790793
H	-2.088676	-0.840614	-1.480140	H	-1.839144	2.506210	1.776528
C	-2.035811	-3.200638	-2.901443	C	-1.569984	4.810242	3.266202
H	-0.907022	-1.494710	-3.586245	H	-0.362650	3.079289	3.713072
H	0.043759	-2.667652	-2.687394	H	0.453848	4.287331	2.732288
H	-1.886124	-3.785792	-3.816032	H	-1.286465	5.358715	4.171793
H	-2.066513	-3.902485	-2.058509	H	-1.718494	5.544881	2.464784
H	-3.020735	-2.722185	-2.970313	H	-2.537199	4.329177	3.457772
O	-11.082820	-0.058910	0.919260	O	-11.424434	0.136195	0.655204
O	11.083057	-0.057854	-0.918711	O	11.448557	0.103106	-0.563882
C	-11.750400	-1.026177	0.202396	C	-12.412371	-0.645619	0.100445
C	-12.675919	-1.802297	0.895521	C	-13.550729	-0.867988	0.871304
C	-11.583294	-1.172594	-1.174748	C	-12.329854	-1.124496	-1.207144
C	-13.438819	-2.740010	0.202392	C	-14.616462	-1.582872	0.328342
H	-12.788901	-1.660127	1.966515	H	-13.588713	-0.476365	1.883834
C	-12.346961	-2.118758	-1.854381	C	-13.399333	-1.844010	-1.735236
H	-10.867411	-0.550944	-1.705003	H	-11.441523	-0.932193	-1.802082
C	-13.275377	-2.905554	-1.172272	C	-14.544504	-2.077109	-0.973329
H	-14.161462	-3.345637	0.743308	H	-15.505023	-1.756056	0.930046
H	-12.219361	-2.233430	-2.927866	H	-13.337587	-2.216839	-2.754544
H	-13.869378	-3.639645	-1.709736	H	-15.375713	-2.636935	-1.393173
C	11.750354	-1.026036	-0.202780	C	12.402161	-0.662920	0.067482
C	12.674665	-1.802740	-0.896836	C	13.586942	-0.895830	-0.626692
C	11.584110	-1.172726	1.174439	C	12.240114	-1.116555	1.376667
C	13.437250	-2.741345	-0.204546	C	14.618744	-1.595913	-0.004758
H	12.786996	-1.660332	-1.967867	H	13.686699	-0.523986	-1.642478
C	12.347426	-2.119770	1.853228	C	13.276760	-1.821450	1.984077
H	10.869142	-0.550593	1.705365	H	11.316165	-0.916445	1.911716
C	13.274655	-2.907164	1.170179	C	14.467586	-2.065038	1.299479
H	14.158973	-3.347439	-0.746167	H	15.543309	-1.777468	-0.546808
H	12.220516	-2.234677	2.926769	H	13.152725	-2.174555	3.004737
H	13.868406	-3.641940	1.706982	H	15.272560	-2.613511	1.780896

2. Molecule **OMe-PV** (PBE0/6-31+G(d)/toluene)

OMe-PV(*a*)				**OMe-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*

C	-3.481089	-0.025482	0.677892	C	3.478149	-0.006092	0.544179
C	-2.529658	-0.032731	-0.361787	C	2.506510	-0.033198	-0.476189
C	-1.174942	-0.024981	-0.075953	C	1.157721	-0.026186	-0.163826
C	-0.730382	-0.011236	1.256921	C	0.739436	0.006929	1.177164
C	-0.000572	-0.028150	-1.041146	C	-0.035257	-0.049734	-1.105474
C	1.173369	-0.012848	-0.075664	C	-1.190142	-0.024444	-0.117442
C	0.728476	-0.003060	1.257088	C	-0.719173	0.007735	1.205987
C	2.528068	-0.005960	-0.361371	C	-2.550269	-0.029223	-0.376339
C	3.479255	0.010836	0.678358	C	-3.480898	-0.001226	0.681621
C	4.895978	0.016508	0.323284	C	-4.904459	-0.003479	0.354603
C	5.947228	0.004438	1.168998	C	-5.938447	0.042659	1.220229
C	7.364078	0.012514	0.815253	C	-7.362233	0.041245	0.895168
C	7.844705	0.070834	-0.501109	C	-7.869929	-0.026989	-0.410544
C	9.206273	0.073494	-0.786794	C	-9.237028	-0.023348	-0.668530
C	10.137921	0.018241	0.256395	C	-10.146772	0.049045	0.392769
C	9.682859	-0.037895	1.578409	C	-9.664623	0.116492	1.704561
H	10.412141	-0.079733	2.382565	H	-10.377080	0.172144	2.522815
C	8.323436	-0.039891	1.844153	C	-8.300056	0.112147	1.942633
H	9.528573	0.120125	-1.821665	H	-9.580612	-0.077627	-1.696173
H	7.147906	0.117903	-1.333738	H	-7.190493	-0.085790	-1.256626
H	7.987981	-0.084647	2.878549	H	-7.943415	0.165810	2.969466
C	-0.006242	1.218122	-1.956441	C	-0.053226	-1.326729	-1.977152
C	-0.010888	2.568154	-1.246857	C	-0.039466	-2.651829	-1.222134
H	-0.885197	1.150207	-2.614436	H	0.812686	-1.285433	-2.654340
H	0.872582	1.157138	-2.615321	H	-0.944768	-1.284149	-2.620139
C	-0.013038	3.742706	-2.221993	C	-0.057144	-3.858559	-2.157058
H	-0.891219	2.639060	-0.593080	H	0.852201	-2.703169	-0.582016
C	-0.015329	5.096057	-1.520081	C	-0.043292	-5.187726	-1.410517
H	0.866082	3.671824	-2.879001	H	-0.948203	-3.808054	-2.799676
H	-0.891739	3.668739	-2.879185	H	0.809236	-3.808274	-2.832568
H	-0.016745	5.922732	-2.239999	H	-0.056404	-6.037890	-2.102409
H	-0.900205	5.207982	-0.881332	H	0.853397	-5.279941	-0.785235
H	0.869275	5.210923	-0.881453	H	-0.915803	-5.279716	-0.751877
C	0.005962	-1.291057	-1.933289	C	-0.052483	1.181715	-2.040476
C	0.013654	-2.628062	-1.199466	C	-0.036449	2.542934	-1.352820
C	0.019734	-3.819666	-2.153734	C	-0.053412	3.701626	-2.346613
C	0.027816	-5.160590	-1.428411	C	-0.035965	5.066110	-1.666826
H	-0.859915	-3.763712	-2.811465	H	0.811887	3.616259	-3.019975
H	0.897849	-3.753787	-2.812587	H	-0.945545	3.620963	-2.984632
H	0.031955	-5.999578	-2.133941	H	-0.048512	5.881036	-2.399896
H	0.913649	-5.257982	-0.788605	H	-0.907306	5.192242	-1.012299
H	-0.855821	-5.267900	-0.787149	H	0.861843	5.187363	-1.048136
H	0.867865	2.644003	-0.591510	H	-0.906563	-2.702793	-0.549070
H	0.893900	-2.684883	-0.544192	H	-0.902887	2.628591	-0.682440
H	-0.865160	-2.694578	-0.543172	H	0.855911	2.625064	-0.716915
H	0.884385	-1.233840	-2.593016	H	-0.944583	1.107954	-2.679875
H	-0.873416	-1.243406	-2.592508	H	0.812807	1.105412	-2.715453
H	2.875979	-0.013618	-1.393971	H	-2.918239	-0.053271	-1.401698
H	-2.877412	-0.041912	-1.394435	H	2.834003	-0.058246	-1.515130
C	3.012095	0.022768	2.008736	C	-2.987625	0.028333	2.002296
C	1.655244	0.015193	2.302888	C	-1.625216	0.033425	2.269619
H	1.326979	0.025647	3.339873	H	-1.276648	0.056700	3.299782
H	3.723527	0.040673	2.829713	H	-3.682790	0.046590	2.837034
C	-1.657368	-0.008664	2.302655	C	1.686785	0.031790	2.204160
C	-3.014202	-0.016641	2.008386	C	3.037587	0.024706	1.883288

H	-3.725846	-0.018752	2.829371	H	3.765276	0.041226	2.689961
H	-1.329271	-0.002294	3.339727	H	1.378993	0.055481	3.247166
H	5.086425	0.028469	-0.749977	H	-5.116296	-0.044128	-0.713972
H	5.756913	-0.017131	2.241936	H	-5.726471	0.089311	2.288317
O	11.483228	0.015713	0.086139	O	-11.495259	0.058841	0.249754
C	11.989170	0.067326	-1.232798	C	-12.027946	-0.003647	-1.058143
H	11.664570	-0.801971	-1.818413	H	-11.710163	0.857388	-1.659436
H	11.681716	0.989328	-1.742102	H	-11.736066	-0.932802	-1.563625
H	13.075704	0.052886	-1.136786	H	-13.112230	0.018160	-0.940577
C	-4.897852	-0.026853	0.322844	C	4.887623	-0.012545	0.161169
C	-5.948546	0.026613	1.167657	C	5.954828	0.039204	0.985184
C	-7.365525	0.026044	0.814313	C	7.363601	0.029952	0.602749
H	-5.088704	-0.069801	-0.749557	H	5.057286	-0.062122	-0.914430
H	-5.757439	0.082428	2.239235	H	5.785551	0.096898	2.060365
C	-7.847562	-0.074762	-0.498960	C	7.816503	-0.064096	-0.728676
C	-8.323522	0.132015	1.840368	C	8.340782	0.117160	1.602933
C	-9.209138	-0.066900	-0.784567	C	9.165082	-0.068333	-1.033017
C	-9.682932	0.141123	1.574690	C	9.704619	0.114024	1.314804
C	-10.139350	0.042336	0.255645	C	10.124641	0.020456	-0.013280
O	-11.484498	0.059394	0.085091	O	11.419630	0.006337	-0.414482
C	-11.991462	-0.032818	-1.231236	H	7.101878	-0.137795	-1.543920
H	-11.698634	-0.977650	-1.706181	H	9.505319	-0.142413	-2.062254
H	-13.077609	0.002260	-1.136279	H	8.027560	0.190628	2.642662
H	-11.653239	0.809062	-1.848349	H	10.419691	0.183891	2.127659
H	-7.151930	-0.164695	-1.329049	C	12.423629	0.088888	0.577193
H	-9.532558	-0.148040	-1.816959	H	13.374589	0.058947	0.043607
H	-7.986952	0.210655	2.872358	H	12.351453	1.028443	1.139333
H	-10.411123	0.224546	2.376594	H	12.368630	-0.759462	1.270924

OMe-PV(*c*)				**OMe-PV(*d*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	-9.674182	-2.006538	-0.064310	C	-9.705716	-1.708761	0.113063
C	-8.312869	-2.259345	-0.024375	C	-8.340269	-1.988234	0.140049
C	-7.361870	-1.222182	-0.065166	C	-7.369455	-1.002339	-0.079465
C	-7.852951	0.088878	-0.149711	C	-7.830582	0.303673	-0.341002
C	-9.216607	0.361607	-0.190652	C	-9.180825	0.599142	-0.371050
C	-10.139748	-0.689675	-0.147992	C	-10.133916	-0.404844	-0.142841
H	-10.396898	-2.817038	-0.031894	H	-10.415541	-2.509663	0.291085
H	-7.969260	-3.289976	0.040691	H	-8.020860	-3.008949	0.341729
H	-7.162872	0.927614	-0.186346	H	-7.120954	1.104547	-0.530261
H	-9.547113	1.392873	-0.256337	H	-9.527520	1.608462	-0.575216
C	-5.942508	-1.562936	-0.018853	C	-5.958003	-1.372090	-0.028642
C	-4.897904	-0.709177	-0.035796	C	-4.896794	-0.545120	-0.131173
C	-3.478779	-1.052648	0.008345	C	-3.484923	-0.917430	-0.085320
C	-1.176685	-0.269661	0.046150	C	-1.167896	-0.183498	-0.013614
C	-0.727724	-1.601754	0.068582	C	-0.746875	-1.524968	-0.008727
C	-0.000045	0.701856	0.014068	C	0.028776	0.763724	-0.016180
C	1.176720	-0.270008	0.024384	C	1.185045	-0.232471	-0.011611
C	0.727937	-1.602055	0.056824	C	0.708598	-1.555278	-0.006351
C	3.478544	-1.050566	0.092496	C	3.469604	-1.061718	0.065990
C	4.898243	-0.707207	0.115156	C	4.895662	-0.747721	0.108226
C	5.940741	-1.558120	0.017829	C	5.922126	-1.618594	0.017174
C	7.360879	-1.218362	0.046619	C	7.348317	-1.307296	0.064438

C	8.309388	-2.231514	-0.188881	C	8.279380	-2.338902	-0.160404
C	9.670637	-1.975421	-0.182717	C	9.645308	-2.110003	-0.136897
C	10.138469	-0.680222	0.065549	C	10.135733	-0.824616	0.118672
C	9.217998	0.345539	0.309763	C	9.232863	0.219060	0.352528
H	9.550560	1.358030	0.513243	H	9.582881	1.224651	0.560933
C	7.854253	0.069815	0.299933	C	7.864124	-0.029398	0.325214
H	10.391748	-2.766583	-0.368062	H	10.352747	-2.915227	-0.314255
H	7.963787	-3.244772	-0.384508	H	7.916199	-3.344896	-0.361670
H	7.165898	0.885959	0.502958	H	7.189753	0.800392	0.519754
C	-2.537397	-0.004031	-0.003102	C	-2.522121	0.111469	-0.073236
H	-2.903155	1.018824	-0.062824	H	-2.866160	1.142557	-0.118932
C	2.537274	-0.002214	0.063920	C	2.550371	0.006190	0.045862
H	2.902992	1.022270	0.080546	H	2.936833	1.022394	0.083939
C	3.002868	-2.376863	0.106468	C	2.966575	-2.377915	0.052455
C	1.643811	-2.656467	0.094005	C	1.602215	-2.628937	0.022020
C	-1.643714	-2.656774	0.078237	C	-1.684383	-2.560653	-0.029074
C	-3.002681	-2.378150	0.055107	C	-3.037090	-2.253235	-0.061636
H	-3.706598	-3.205699	0.061449	H	-3.758394	-3.065345	-0.088680
H	-1.302798	-3.689553	0.095497	H	-1.364849	-3.600365	-0.032291
H	1.302840	-3.688876	0.125966	H	1.239860	-3.654518	0.032874
H	3.707384	-3.202992	0.147411	H	3.653421	-3.219151	0.085246
H	5.739053	-2.621718	-0.109340	H	5.701031	-2.677222	-0.118784
H	5.099433	0.360235	0.207891	H	5.117166	0.314647	0.212238
H	-5.096503	0.361517	-0.086395	H	-5.074159	0.523951	-0.249182
H	-5.744034	-2.633195	0.036264	H	-5.780649	-2.437367	0.119500
C	0.090885	1.585731	1.283810	C	0.124343	1.621472	1.271148
C	-0.993788	2.638012	1.492990	C	-0.941469	2.690944	1.489729
H	1.067625	2.089097	1.270982	H	1.110999	2.105271	1.277631
H	0.112869	0.916195	2.154738	H	0.124073	0.935205	2.129253
C	-0.728062	3.495799	2.728770	C	-0.672416	3.518756	2.745081
H	-1.066693	3.294600	0.614064	H	-0.991758	3.366044	0.623338
H	-1.972186	2.153340	1.604621	H	-1.930419	2.223871	1.581384
C	-1.808176	4.544372	2.968828	C	-1.733978	4.584056	2.994055
H	-0.645946	2.843963	3.610097	H	-0.613381	2.848190	3.614142
H	0.248180	3.990763	2.623555	H	0.314712	3.995754	2.660310
H	-1.592500	5.146401	3.858998	H	-1.516437	5.163959	3.898352
H	-1.891704	5.229415	2.115711	H	-1.794000	5.287267	2.153863
H	-2.789292	4.075371	3.114122	H	-2.725912	4.132340	3.119058
C	-0.090649	1.527577	-1.294465	C	-0.031314	1.615715	-1.309447
C	0.993625	2.569989	-1.549916	C	1.075936	2.641021	-1.533590
H	-1.067816	2.030139	-1.305553	H	-0.998096	2.137908	-1.320781
H	-0.111141	0.819286	-2.134208	H	-0.056934	0.924071	-2.162833
C	0.731425	3.367548	-2.826146	C	0.843114	3.467603	-2.796975
H	1.062818	3.267922	-0.703078	H	1.149549	3.321283	-0.672897
H	1.972881	2.081712	-1.635004	H	2.046364	2.135251	-1.617793
C	1.810683	4.405667	-3.111234	C	1.945422	4.489458	-3.050919
H	0.654365	2.674379	-3.675815	H	0.761641	2.792304	-3.660520
H	-0.246212	3.864867	-2.748700	H	-0.125371	3.982583	-2.720148
H	1.597774	4.964195	-4.029969	H	1.753355	5.069357	-3.960965
H	1.889265	5.130713	-2.291349	H	2.029229	5.197181	-2.216550
H	2.793255	3.932244	-3.229830	H	2.919813	3.999101	-3.168284
O	11.484838	-0.518158	0.053304	O	11.485094	-0.689247	0.122964
O	-11.486239	-0.532106	-0.182732	O	-11.431143	-0.013875	-0.194793
C	-12.002448	0.781110	-0.266773	C	12.026485	0.592023	0.374395
H	-11.708292	1.381519	0.603296	H	11.743948	0.955897	1.370276

H	-11.673320	1.280885	-1.186518	H	13.109837	0.473182	0.327354
H	-13.088042	0.675059	-0.282016	H	11.706984	1.315999	-0.385714
C	12.003680	0.773879	0.296957	C	-12.429188	-0.990666	0.023913
H	11.725462	1.133530	1.295587	H	-13.383035	-0.468515	-0.062669
H	13.088561	0.676388	0.237593	H	-12.379957	-1.785904	-0.730531
H	11.661205	1.490261	-0.460339	H	-12.344306	-1.429230	1.026156

3. Molecule **NH_2-PV**(PBE0/6-31+G(d)/toluene)

NH_2-PV(*a*)				**NH_2-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	-9.687221	0.045097	1.500320	C	-9.677462	-1.950905	-0.034628
C	-8.324451	0.042785	1.763174	C	-8.312324	-2.200476	-0.015355
C	-7.365554	-0.001024	0.737127	C	-7.362641	-1.167790	-0.091308
C	-7.851831	-0.045484	-0.582329	C	-7.860744	0.144141	-0.191548
C	-9.209214	-0.043102	-0.857639	C	-9.220682	0.406204	-0.211082
C	-10.157174	0.002204	0.179895	C	-10.159339	-0.637826	-0.133304
H	-10.397450	0.084851	2.323853	H	-10.380076	-2.779214	0.031611
H	-7.988901	0.075679	2.798269	H	-7.967509	-3.230232	0.060860
H	-7.156867	-0.084943	-1.417087	H	-7.173216	0.983291	-0.258909
H	-9.549032	-0.072858	-1.891141	H	-9.569788	1.434432	-0.284484
C	-5.949814	0.001003	1.086755	C	-5.943844	-1.503950	-0.063978
C	-4.898043	-0.018707	0.240427	C	-4.899203	-0.649465	-0.099702
C	-3.481710	-0.015691	0.595886	C	-3.480147	-0.993851	-0.072858
C	-1.174446	-0.005590	-0.156841	C	-1.176890	-0.213598	-0.012590
C	-0.729388	-0.003723	1.175992	C	-0.727638	-1.545757	-0.032888
C	-0.000015	0.000288	-1.122140	C	0.000187	0.758300	-0.012773
C	1.174430	0.005924	-0.156857	C	1.177179	-0.213451	-0.033361
C	0.729384	0.003692	1.175988	C	0.727851	-1.545668	-0.043353
C	3.481703	0.015813	0.595858	C	3.480354	-0.995016	0.015381
C	4.898031	0.018864	0.240383	C	4.899125	-0.651182	0.058937
C	5.949797	-0.001578	1.0867006	C	5.943557	-1.506670	0.063013
C	7.365543	0.000475	0.737099	C	7.361926	-1.170581	0.107936
C	8.324418	-0.043825	1.763149	C	8.311176	-2.206429	0.103468
C	9.687197	-0.046096	1.500323	C	9.675869	-1.957316	0.146041
C	10.157184	-0.002663	0.179922	C	10.157688	-0.641476	0.195992
C	9.209242	0.043092	-0.857616	C	9.219524	0.405896	0.199852
H	9.549080	0.073226	-1.891100	H	9.568793	1.436234	0.231633
C	7.851853	0.045399	-0.582330	C	7.860014	0.144258	0.157873
H	10.397408	-0.086224	2.323853	H	10.378337	-2.788365	0.136784
H	7.988843	-0.077119	2.798222	H	7.966354	-3.238359	0.067044
H	7.156906	0.085106	-1.417092	H	7.172765	0.986281	0.165364
C	-0.006180	1.254773	-2.025967	C	-2.537476	0.053951	-0.052772
C	-0.013357	2.598375	-1.304345	H	-2.902825	1.078421	-0.078432
H	-0.884688	1.191897	-2.685136	C	2.537727	0.053016	0.014847
H	0.873298	1.200895	-2.684647	H	2.903002	1.076617	0.064872
C	-0.019181	3.781447	-2.269129	N	-11.519728	-0.367783	-0.092528
H	-0.893497	2.661219	-0.649520	N	11.519277	-0.374849	0.178091
C	-0.026606	5.128708	-1.555588	C	3.003564	-2.320892	-0.019784
H	0.860336	3.719405	-2.926528	C	1.644600	-2.600075	-0.042032
H	-0.897502	3.710165	-2.927156	C	-1.644382	-2.599834	-0.058486

H	-0.030677	5.961609	-2.268347	C	-3.003392	-2.320185	-0.072236
H	-0.912234	5.231850	-0.916395	H	-3.707387	-3.147399	-0.097319
H	0.857244	5.241177	-0.915475	H	-1.303932	-3.632827	-0.077106
C	0.006141	-1.254012	-2.026252	H	1.304169	-3.633209	-0.050521
C	0.013366	-2.597769	-1.304931	H	3.707479	-3.148536	-0.018643
C	0.019196	-3.780631	-2.269977	H	12.116446	-1.122051	0.506551
C	0.026671	-5.128047	-1.556731	H	11.795557	0.520430	0.558755
H	-0.860338	-3.718463	-2.927342	H	5.742125	-2.577519	0.029142
H	0.897501	-3.709181	-2.928008	H	5.098579	0.420107	0.090827
H	0.030745	-5.960792	-2.269673	H	-5.098746	0.421236	-0.147144
H	0.912316	-5.231308	-0.917583	H	-5.742114	-2.573545	-0.002769
H	-0.857161	-5.240677	-0.916622	H	-11.804739	0.511002	-0.503944
H	0.865605	2.670285	-0.648842	H	-12.126168	-1.127146	-0.372545
H	0.893522	-2.660742	-0.650141	C	0.090572	1.600181	1.285237
H	-0.865581	-2.669851	-0.649426	C	-0.993248	2.646251	1.527565
H	0.884629	-1.190963	-2.685430	H	1.067960	2.102487	1.290371
H	-0.873359	-1.199992	-2.684891	H	0.110572	0.902378	2.133745
C	-2.528993	-0.011734	-0.443070	C	-0.729829	3.461015	2.792592
H	-2.876200	-0.012221	-1.475992	H	-1.062991	3.332652	0.671389
C	2.528972	0.012137	-0.443094	H	-1.972527	2.159400	1.619953
H	2.876177	0.012915	-1.476017	C	-1.808593	4.503203	3.064511
N	-11.514307	0.066215	-0.100860	H	-0.652182	2.779425	3.651547
N	11.514316	-0.066573	-0.100828	H	0.247876	3.957011	2.707580
C	3.014030	0.016192	1.926385	H	-1.594842	5.074222	3.975373
C	1.657164	0.009631	2.221035	H	-1.887733	5.216974	2.234830
C	-1.657158	-0.009909	2.221050	H	-2.791184	4.031674	3.190291
C	-3.014023	-0.016388	1.926414	C	-0.090070	1.626548	-1.293356
H	-3.725654	-0.023347	2.747454	C	0.994647	2.676276	-1.514705
H	-1.329455	-0.010773	3.258357	H	-1.067044	2.129650	-1.287793
H	1.329478	0.010225	3.258348	H	-0.110987	0.946117	-2.155837
H	3.725666	0.023002	2.747423	C	0.731899	3.516345	-2.763215
H	12.130669	0.235760	0.641746	H	1.064969	3.345309	-0.644957
H	11.795147	0.307223	-0.997560	H	1.973504	2.190470	-1.616754
H	5.757187	-0.025624	2.159447	C	1.811827	4.562432	-3.014801
H	5.088735	0.035979	-0.832810	H	0.653141	2.852022	-3.635494
H	-5.088756	-0.035119	-0.832775	H	-0.245165	4.011767	-2.668068
H	-5.757224	0.024393	2.159519	H	1.598500	5.151604	-3.914129
H	-11.795096	-0.307187	-0.997771	H	1.892073	5.259565	-2.171200
H	-12.130658	-0.236511	0.641557	H	2.793815	4.092307	-3.150208

4. Molecule **NPh_2-PV** (PBE0/6-31+G(d)/toluene)

NPh_2-PV(*a*)				**NPh_2-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*

C	9.307159	0.710003	-0.653422	C	-9.315302	-1.151469	-0.467316
C	7.949465	0.940246	-0.802160	C	-7.956009	-1.391932	-0.581688
C	6.993049	0.182970	-0.100726	C	-7.003188	-0.439352	-0.175841
C	7.478642	-0.818997	0.756568	C	-7.494141	0.765932	0.354522
C	8.837270	-1.049053	0.923937	C	-8.853896	1.011779	0.486602
C	9.777020	-0.287006	0.217738	C	-9.789889	0.055070	0.073401
H	10.020200	1.302410	-1.220109	H	-10.026168	-1.901928	-0.802191
H	7.630210	1.713052	-1.496334	H	-7.633583	-2.335511	-1.013968
H	6.769446	-1.422811	1.319765	H	-6.787648	1.524879	0.685647
H	9.176407	-1.824054	1.605593	H	-9.196937	1.950615	0.912377
C	5.552596	0.378488	-0.219528	C	-5.561366	-0.633317	-0.277869
C	3.477367	1.530289	-1.050645	C	-4.918779	-1.731627	-0.728522
C	1.175414	0.904892	-0.643688	C	-3.475520	-1.924873	-0.831135
C	0.729218	2.028696	-1.366780	C	-1.177659	-1.199089	-0.553799
C	0.000024	0.092911	-0.122777	C	-0.725799	-2.433283	-1.063757
C	-1.175369	0.904945	-0.643601	C	1.177769	-1.213485	-0.511843
C	-0.729175	2.028732	-1.366722	C	0.729308	-2.442003	-1.038188
C	-3.477326	1.530460	-1.050357	C	3.478001	-1.913665	-0.835342
C	-5.552567	0.378309	-0.219732	C	4.921611	-1.706067	-0.764026
C	-6.993025	0.182874	-0.100860	C	5.565748	-0.627515	-0.269395
C	-7.949454	0.940670	-0.801715	C	7.008066	-0.421789	-0.198140
C	-9.307152	0.710472	-0.652948	C	7.501252	0.755434	0.389945
C	-9.777005	-0.287015	0.217670	C	8.861590	1.009629	0.498475
C	-8.837241	-1.049579	0.923294	C	9.795515	0.090739	0.002709
H	-9.176368	-1.824956	1.604527	C	9.318414	-1.087134	-0.596092
C	-7.478612	-0.819563	0.755887	H	10.027418	-1.807171	-0.995416
H	-10.020203	1.303288	-1.219193	C	7.958912	-1.336291	-0.688139
H	-7.630207	1.713859	-1.495466	H	9.206699	1.925889	0.969276
H	-6.769406	-1.423790	1.318629	H	6.796463	1.484560	0.785356
C	0.000075	0.009998	1.421074	H	7.633959	-2.255202	-1.168848
C	0.000078	1.343587	2.161091	C	-2.534408	-0.958063	-0.419663
H	0.878999	-0.576074	1.727971	C	2.533978	-0.945436	-0.433086
H	-0.878815	-0.576095	1.728026	H	2.878623	0.019953	-0.074332
C	0.000110	1.172121	3.678033	N	-11.171938	0.296043	0.191563
H	0.879652	1.931147	1.863366	N	11.178928	0.340013	0.096824
C	0.000112	2.501108	4.425008	C	-11.693072	1.587081	-0.056155
H	-0.878789	0.582908	3.977768	C	-11.233727	2.343426	-1.142619
H	0.879034	0.582926	3.977732	C	-12.679388	2.125485	0.780281
H	0.000137	2.352168	5.511039	C	-11.746920	3.615332	-1.378738
H	0.884886	3.097362	4.169672	H	-10.473319	1.928813	-1.798883
H	-0.884686	3.097342	4.169710	C	-13.199463	3.391406	0.526905
C	-0.000031	-1.344782	-0.691399	H	-13.036696	1.545760	1.627058
C	-0.000139	-1.461204	-2.212128	C	-12.735135	4.146740	-0.549749
C	-0.000206	-2.911435	-2.688953	H	-11.379831	4.188535	-2.226642
C	-0.000312	-3.035846	-4.208392	H	-13.964813	3.794109	1.185892
H	0.878765	-3.429544	-2.278554	H	-13.138683	5.137446	-0.740813
H	-0.879144	-3.429503	-2.278435	C	12.070256	-0.715787	0.398220
H	-0.000358	-4.084992	-4.526115	C	13.298037	-0.821142	-0.268917
H	-0.885128	-2.555059	-4.643700	C	11.739181	-1.669233	1.369972
H	0.884468	-2.555101	-4.643820	C	14.176706	-1.855809	0.038261
H	-0.879520	1.931128	1.863401	H	13.558913	-0.087596	-1.026896
H	-0.879787	-0.945698	-2.622012	C	12.616528	-2.710202	1.659102
H	0.879475	-0.945739	-2.622132	H	10.792105	-1.589241	1.896646
H	-0.878883	-1.868212	-0.286715	C	13.841516	-2.809370	0.999633
H	0.878864	-1.868234	-0.286837	H	15.125167	-1.922998	-0.489124

C	2.525417	0.654948	-0.486962	H	12.344063	-3.441135	2.416554
H	2.853039	-0.221987	0.067343	H	14.527029	-3.619709	1.232516
C	-2.525370	0.655076	-0.486747	C	11.679122	1.649287	-0.093704
H	-2.852980	-0.221808	0.067645	C	12.685814	2.154038	0.739686
N	11.157943	-0.516377	0.369407	C	11.175781	2.458658	-1.120820
N	-11.157929	-0.516347	0.369371	C	13.180083	3.440229	0.542618
C	11.647656	-1.835044	0.517136	H	13.077908	1.533224	1.540666
C	11.140193	-2.874231	-0.273755	C	11.663825	3.749437	-1.300248
C	12.650245	-2.118511	1.453579	H	10.400193	2.070317	-1.775326
C	11.621778	-4.170921	-0.121188	C	12.670547	4.248389	-0.473555
H	10.367394	-2.659459	-1.006853	H	13.960983	3.816897	1.198873
C	13.138058	-3.415112	1.587983	H	11.262190	4.363818	-2.102409
H	13.045215	-1.317599	2.072671	H	13.054488	5.254249	-0.620605
C	12.625419	-4.450331	0.806456	C	-12.045877	-0.750964	0.565126
H	11.217557	-4.965612	-0.743522	C	-11.686086	-1.650964	1.576557
H	13.916311	-3.617984	2.319679	C	-13.285571	-0.899542	-0.070520
H	13.004004	-5.462762	0.918304	C	-12.547349	-2.683992	1.934515
C	-11.647740	-1.835047	0.516481	H	-10.729041	-1.536295	2.078396
C	-12.650248	-2.118901	1.452893	C	-14.147688	-1.925492	0.304703
C	-11.140460	-2.873875	-0.274999	H	-13.568183	-0.206656	-0.858488
C	-13.138161	-3.415527	1.586693	C	-13.784028	-2.826873	1.305300
H	-13.045076	-1.318268	2.072437	H	-12.252917	-3.373960	2.721553
C	-11.622143	-4.170599	-0.123038	H	-15.105507	-2.027314	-0.199733
H	-10.367726	-2.658797	-1.008074	H	-14.456777	-3.630708	1.591808
C	-12.625703	-4.450392	0.804580	C	-0.001316	-0.311202	-0.155358
H	-13.916350	-3.618701	2.318374	C	0.098662	0.977747	-1.009874
H	-11.218065	-4.965009	-0.745823	C	-0.987042	2.034270	-0.828757
H	-13.004363	-5.462847	0.915956	H	0.130825	0.675456	-2.065815
C	-12.061319	0.571522	0.383168	H	1.073878	1.440610	-0.804435
C	-13.282994	0.487013	-0.297511	C	-0.713415	3.285746	-1.660893
C	-11.748888	1.746649	1.079180	H	-1.962934	1.625346	-1.120725
C	-14.174086	1.555749	-0.274282	H	-1.070822	2.322810	0.228967
H	-13.529557	-0.420159	-0.842469	C	-1.796183	4.348050	-1.511027
C	-12.638566	2.816896	1.083340	H	0.259497	3.708368	-1.371267
H	-10.806288	1.815781	1.615390	H	-0.619737	3.002522	-2.718915
C	-13.857519	2.728646	0.411106	H	-1.575475	5.234589	-2.116550
H	-15.117719	1.473761	-0.808196	H	-2.773829	3.963924	-1.827766
H	-12.380622	3.721373	1.628880	H	-1.890437	4.673058	-0.467208
H	-14.552820	3.563684	0.421824	C	-0.104533	-0.025345	1.364618
C	12.061416	0.571429	0.382564	C	0.976098	0.845863	1.997216
C	11.749140	1.746928	1.078018	H	-0.133397	-0.993147	1.883963
C	13.283016	0.486494	-0.298199	H	-1.082105	0.440486	1.550943
C	12.638893	2.817115	1.081550	C	0.694925	1.126838	3.472176
H	10.806601	1.816397	1.614290	H	1.953511	0.353319	1.913936
C	14.174184	1.555180	-0.275598	H	1.059787	1.803338	1.463021
H	13.529460	-0.420967	-0.84272	C	1.773071	1.979288	4.131223
C	13.857770	2.728443	0.409235	H	-0.279494	1.627448	3.566996
H	12.381068	3.721884	1.626662	H	0.600747	0.172718	4.009922
H	15.117756	1.472858	-0.809569	H	1.546511	2.167515	5.186937
H	14.553131	3.563437	0.419461	H	2.751621	1.485416	4.084163
C	-3.010746	2.646361	-1.772791	H	1.868798	2.952161	3.632802
C	-1.653808	2.903922	-1.935350	H	-2.882372	-0.026178	0.016307
C	1.653847	2.903819	-1.935520	H	4.977340	0.195805	0.135453
C	3.010786	2.646186	-1.773083	H	5.512208	-2.535388	-1.153236
H	-3.738548	3.324985	-2.213331	H	-4.971715	0.221389	0.053492

H	-1.329286	3.775625	-2.499093	H	-5.509785	-2.585105	-1.060534
H	1.329320	3.775517	-2.499267	C	1.644940	-3.409972	-1.448337
H	3.738586	3.324757	-2.213709	C	3.003823	-3.140821	-1.336805
C	-4.919093	1.338791	-0.926112	C	-1.638677	-3.405019	-1.471039
H	-5.517077	2.072278	-1.466842	C	-2.998333	-3.140598	-1.357145
H	-4.955882	-0.341228	0.340832	H	-1.300541	-4.360301	-1.866025
C	4.919133	1.338551	-0.926487	H	-3.717752	-3.893289	-1.673594
H	5.517119	2.071630	-1.467766	H	1.309458	-4.360393	-1.857137
H	4.955903	-0.340575	0.341638	H	3.725275	-3.891532	-1.653354

5. Molecule **NPh_2-PE** (PBE0/6-31+G(d)/toluene)

NPh_2-PE(a)				**NPh_2-PE(b)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	9.750121	0.905385	-0.940749	C	-9.748591	-1.447004	-0.638890
C	8.390388	1.090632	-1.133679	C	-8.386860	-1.680808	-0.746412
C	7.445817	0.361365	-0.388255	C	-7.450147	-0.723996	-0.314283
C	7.923420	-0.557815	0.563886	C	-7.937533	0.475182	0.237092
C	9.282805	-0.735187	0.766847	C	-9.298943	0.705187	0.356846
C	10.220631	-0.008637	0.015699	C	-10.228810	-0.250763	-0.082343
H	10.460661	1.470752	-1.536787	H	-10.453106	-2.195020	-0.990909
H	8.045032	1.798788	-1.881801	H	-8.033802	-2.610218	-1.184579
H	7.212670	-1.125189	1.158364	H	-7.232877	1.224526	0.586984
H	9.627913	-1.441258	1.516622	H	-9.651908	1.633260	0.797213
C	6.052474	0.548604	-0.590887	C	-6.054739	-0.962127	-0.431948
C	4.857545	0.712044	-0.766109	C	-4.858183	-1.168947	-0.535432
C	3.463829	0.902961	-0.969552	C	-3.462414	-1.409731	-0.656264
C	1.173770	0.374697	-0.420369	C	-1.175950	-0.689517	-0.331386
C	0.729697	1.297286	-1.385695	C	-0.727791	-1.904056	-0.885029
C	0.000004	-0.292530	0.277128	C	1.175762	-0.714145	-0.277917
C	-1.173763	0.374680	-0.420384	C	0.728009	-1.918982	-0.852601
C	-0.729693	1.297273	-1.385704	C	3.462460	-1.422593	-0.626060
C	-3.463822	0.902904	-0.969597	C	4.858102	-1.172237	-0.524870
C	-4.857539	0.711971	-0.766171	C	6.054552	-0.956531	-0.439938
C	-6.052468	0.548534	-0.590937	C	7.449865	-0.708807	-0.342758
C	-7.445813	0.361314	-0.388296	C	7.936936	0.501423	0.184181
C	-8.390380	1.090549	-1.133758	C	9.298344	0.740767	0.284101
C	-9.750114	0.905322	-0.940815	C	10.228369	-0.216796	-0.151248
C	-10.220630	-0.008655	0.015673	C	9.748366	-1.424078	-0.683659
C	-9.282809	-0.735175	0.766856	H	10.452891	-2.173556	-1.032535
H	-9.627920	-1.441203	1.516668	C	8.386819	-1.666967	-0.771374
C	-7.923423	-0.557816	0.563891	H	9.651187	1.677477	0.705881
H	-10.460650	1.470662	-1.536883	H	7.232233	1.252277	0.530729
H	-8.045019	1.798660	-1.881920	H	8.033888	-2.604903	-1.191091
H	-7.212675	-1.125160	1.158401	C	-2.534536	-0.450924	-0.198627
C	-0.000008	-0.009781	1.797525	C	2.534197	-0.457350	-0.182986
C	-0.000023	1.460013	2.205001	H	2.909717	0.479941	0.216614
H	0.878797	-0.507739	2.232765	N	-11.609624	-0.015611	0.032560
H	-0.878809	-0.507754	2.232754	N	11.609094	0.027340	-0.056120

C	-0.000036	1.646242	3.720265	C	-12.131024	1.286441	-0.158136
H	0.879735	1.962443	1.779389	C	-11.671411	2.089184	-1.209974
C	-0.000052	3.112589	4.137328	C	-13.120242	1.784398	0.699115
H	-0.878996	1.142953	4.148546	C	-12.185905	3.369644	-1.390501
H	0.878926	1.142968	4.148559	H	-10.910440	1.704487	-1.883627
H	-0.000062	3.220122	5.228203	C	-13.641601	3.059676	0.501243
H	0.884824	3.633119	3.750565	H	-13.478527	1.166307	1.517879
H	-0.884932	3.633103	3.750551	C	-13.175742	3.862175	-0.540041
C	0.000016	-1.824150	0.062664	H	-11.818897	3.980199	-2.211864
C	0.000026	-2.297051	-1.387401	H	-14.409108	3.431870	1.175415
C	0.000039	-3.819133	-1.505305	H	-13.580281	4.859820	-0.687929
C	0.000049	-4.301851	-2.951355	C	12.500910	-1.027565	0.253734
H	0.879000	-4.224264	-0.983202	C	13.711367	-1.156351	-0.438667
H	-0.878919	-4.224279	-0.983209	C	12.188151	-1.949651	1.260558
H	0.000058	-5.396468	-3.009614	C	14.592819	-2.186235	-0.122883
H	-0.884818	-3.938940	-3.488794	H	13.957214	-0.444777	-1.222256
H	0.884915	-3.938926	-3.488787	C	13.067371	-2.986528	1.558486
H	-0.879784	1.962428	1.779376	H	11.254011	-1.849215	1.806620
H	-0.879709	-1.894280	-1.908334	C	14.275760	-3.110028	0.872785
H	0.879759	-1.894265	-1.908327	H	15.528622	-2.272935	-0.669560
H	-0.878755	-2.236775	0.579646	H	12.810297	-3.694158	2.342873
H	0.878789	-2.236762	0.579653	H	14.963190	-3.916758	1.112490
C	2.525828	0.174063	-0.208835	C	12.121338	1.329262	-0.270971
H	2.883025	-0.535293	0.534109	C	13.117509	1.844250	0.567973
C	-2.525821	0.174023	-0.208867	C	11.645771	2.114776	-1.328699
H	-2.883015	-0.535340	0.534071	C	13.629992	3.119215	0.346348
N	11.599222	-0.191797	0.216744	H	13.488203	1.239585	1.391226
N	-11.599225	-0.191794	0.216727	C	12.151585	3.395132	-1.533005
C	12.112588	-1.474553	0.525046	H	10.879282	1.716796	-1.988233
C	11.656212	-2.606792	-0.161667	C	13.148355	3.904584	-0.700790
C	13.090548	-1.624701	1.516162	H	14.403084	3.504719	1.006512
C	12.162967	-3.865425	0.148158	H	11.772221	3.992164	-2.358685
H	10.903773	-2.494712	-0.937670	H	13.546058	4.902049	-0.867265
C	13.604323	-2.884900	1.808112	C	-12.492225	-1.079771	0.336913
H	13.446011	-0.749497	2.053246	C	-12.162583	-2.015505	1.325622
C	13.141744	-4.013042	1.130975	C	-13.710346	-1.204373	-0.342722
H	11.798745	-4.734562	-0.394097	C	-13.032824	-3.061454	1.618153
H	14.363153	-2.985062	2.580282	H	-11.222424	-1.918520	1.861893
H	13.540343	-4.996340	1.365655	C	-14.582643	-2.243591	-0.032161
C	-12.112610	-1.474554	0.524985	H	-13.969326	-0.482240	-1.112290
C	-13.090478	-1.624740	1.516187	C	-14.248820	-3.180838	0.945282
C	-11.656351	-2.606760	-0.161862	H	-12.762633	-3.779621	2.388426
C	-13.604273	-2.884941	1.808093	H	-15.524567	-2.326830	-0.568772
H	-13.445851	-0.749565	2.053375	H	-14.929172	-3.994753	1.180854
C	-12.163127	-3.865395	0.147915	C	-0.000233	0.178299	0.107512
H	-10.903988	-2.494651	-0.937934	C	0.109508	1.499214	-0.696210
C	-13.141810	-4.013049	1.130821	C	-0.971772	2.552722	-0.475897
H	-14.363028	-2.985133	2.580333	H	0.143839	1.238730	-1.763091
H	-11.798997	-4.734506	-0.394446	H	1.086182	1.947852	-0.468199
H	-13.540425	-4.996350	1.365464	C	-0.686470	3.836045	-1.254089
C	-12.488371	0.905116	0.114577	H	-1.948756	2.162313	-0.788369
C	-13.710149	0.764182	-0.555234	H	-1.058224	2.797525	0.592416
C	-12.162188	2.140520	0.688315	C	-1.762793	4.898383	-1.062724
C	-14.589473	1.839608	-0.642203	H	0.288192	4.239363	-0.943688
H	-13.966431	-0.191676	-1.004063	H	-0.591333	3.597012	-2.322818

C	-13.039598	3.215613	0.582102	H	-1.533612	5.808158	-1.629377
H	-11.219193	2.252909	1.216532	H	-2.741779	4.534619	-1.398577
C	-14.259192	3.072315	-0.079536	H	-1.858641	5.179228	-0.006356
H	-15.534203	1.714347	-1.165550	C	-0.109905	0.404955	1.637080
H	-12.772056	4.168066	1.033043	C	0.971952	1.247341	2.305921
H	-14.945012	3.911841	-0.154786	H	-0.144453	-0.581965	2.118809
C	12.488389	0.905090	0.114523	H	-1.086417	0.867317	1.836437
C	12.162224	2.140535	0.688182	C	0.688724	1.467077	3.790960
C	13.710163	0.764090	-0.555279	H	1.948930	0.757896	2.203202
C	13.039651	3.215608	0.581898	H	1.057170	2.226017	1.812306
H	11.219228	2.252972	1.216388	C	1.765984	2.292248	4.485404
C	14.589505	1.839495	-0.642318	H	-0.285832	1.963322	3.904825
H	13.966426	-0.191803	-1.004045	H	0.594376	0.491646	4.288972
C	14.259243	3.072245	-0.079731	H	1.538321	2.436187	5.547833
H	12.772126	4.168096	1.032775	H	2.744893	1.801601	4.418112
H	15.534234	1.714186	-1.165657	H	1.861098	3.284935	4.027698
H	14.945078	3.911754	-0.155035	H	-2.910566	0.457631	0.262127
C	-3.007208	1.824465	-1.934418	C	-2.996562	-2.609521	-1.230446
C	-1.648741	2.023898	-2.144834	C	-1.635892	-2.861881	-1.339195
C	1.648742	2.023930	-2.144807	H	-1.290612	-3.799345	-1.768656
C	3.007213	1.824517	-1.934374	H	-3.719084	-3.341902	-1.579133
H	-3.737103	2.380965	-2.515475	C	1.636476	-2.881582	-1.295814
H	-1.316312	2.739218	-2.893402	C	2.997065	-2.634342	-1.174971
H	1.316312	2.739251	-2.893375	H	3.719877	-3.371000	-1.513914
H	3.737104	2.381032	-2.515422	H	1.291542	-3.813256	-1.737965

6. Molecule **NBu_2-PV** (PBE0/6-31+G(d)/toluene)

NBu_2-PV(*a*)				**NBu_2-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	9.320302	-0.955408	-0.148037	C	-9.680826	-1.797485	-0.132689
C	7.964499	-1.226471	-0.087813	C	-8.319455	-2.051791	-0.076228
C	6.992784	-0.257663	-0.393781	C	-7.356770	-1.046061	-0.261986
C	7.478182	1.008019	-0.759308	C	-7.850848	0.241098	-0.530769
C	8.832304	1.299496	-0.825106	C	-9.208483	0.511534	-0.597736
C	9.807139	0.318333	-0.533952	C	-10.175402	-0.499462	-0.388317
H	10.009989	-1.749790	0.114750	H	-10.367518	-2.616807	0.052420
H	7.659426	-2.225458	0.214030	H	-7.988322	-3.067721	0.133518
H	6.766581	1.797435	-0.996837	H	-7.159849	1.059566	-0.717619
H	9.126504	2.305238	-1.103658	H	-9.511325	1.521500	-0.850045
C	5.556308	-0.489263	-0.341759	C	-5.941816	-1.382199	-0.177127
C	3.480897	-1.860103	0.035430	C	-4.894391	-0.531608	-0.238850
C	1.176515	-1.148957	-0.183412	C	-3.477435	-0.875229	-0.160791
C	0.729309	-2.431758	0.189786	C	-1.176788	-0.095158	-0.030129
C	0.000738	-0.223274	-0.455460	C	-0.727519	-1.427576	-0.018834
C	-1.175521	-1.148611	-0.184297	C	0.000007	0.876701	0.000069
C	-0.728971	-2.431565	0.189170	C	1.176808	-0.095150	0.030325
C	-3.480247	-1.859084	0.032937	C	0.727545	-1.427571	0.019143
C	-5.555401	-0.487025	-0.342181	C	3.477458	-0.875199	0.161050
C	-6.991930	-0.255583	-0.394026	C	4.894412	-0.531569	0.239077
C	-7.963398	-1.225662	-0.091326	C	5.941844	-1.382135	0.177139
C	-9.319267	-0.954945	-0.151168	C	7.356801	-1.046001	0.261961

C	-9.806514	0.319729	-0.533411	C	8.319479	-2.051749	0.076279
C	-8.831943	1.302266	-0.820847	C	9.680854	-1.797455	0.132740
H	-9.126463	2.308836	-1.096074	C	10.175446	-0.499419	0.388278
C	-7.477699	1.011083	-0.755632	C	9.208530	0.511604	0.597595
H	-10.008711	-1.750475	0.108759	H	9.511368	1.521594	0.849808
H	-7.658088	-2.225502	0.207419	C	7.850895	0.241176	0.530635
H	-6.766342	1.801572	-0.990324	H	10.367531	-2.616805	-0.052296
C	0.001349	0.291438	-1.913245	H	7.988340	-3.067692	-0.133395
C	0.001672	-0.778744	-2.999867	H	7.159910	1.059678	0.717386
H	0.880569	0.940007	-2.042278	C	-2.534763	0.172311	-0.121854
H	-0.877660	0.940157	-2.042951	H	-2.898255	1.196490	-0.172979
C	0.002146	-0.185361	-4.406409	C	2.534782	0.172333	0.122028
H	0.881287	-1.426306	-2.880015	H	2.898268	1.196519	0.173062
C	0.002467	-1.248711	-5.498941	N	-11.538139	-0.255336	-0.426159
H	-0.876806	0.464517	-4.527518	N	11.538181	-0.255311	0.426148
H	0.881209	0.464472	-4.526953	C	3.001423	-2.201577	0.130029
H	0.002776	-0.798683	-6.498595	C	1.643798	-2.481425	0.065218
H	0.887235	-1.892828	-5.422343	C	-1.643767	-2.481438	-0.064810
H	-0.882363	-1.892806	-5.422883	C	-3.001394	-2.201603	-0.129636
C	0.000535	0.996750	0.493883	H	-3.704810	-3.028514	-0.175608
C	-0.000135	0.681625	1.986122	H	-1.303509	-3.514713	-0.062507
C	-0.000267	1.939829	2.850594	H	1.303543	-3.514702	0.063017
C	-0.000877	1.633489	4.344063	H	3.704844	-3.028480	0.176107
H	0.878924	2.552128	2.602220	H	5.743850	-2.445420	0.038444
H	-0.879079	2.552405	2.601557	H	5.092221	0.535276	0.345930
H	-0.000966	2.551491	4.943307	H	-5.092214	0.535250	-0.345548
H	-0.885859	1.049985	4.626725	H	-5.743823	-2.445503	-0.038579
H	0.883716	1.049718	4.627391	C	0.045511	1.731795	1.291726
H	-0.878070	-1.426240	-2.880593	C	-1.046353	2.779472	1.486025
H	-0.879938	0.071830	2.234209	H	1.022071	2.234620	1.325521
H	0.879255	0.071527	2.234932	H	0.036396	1.042467	2.147332
H	-0.878302	1.612992	0.252440	C	-0.827291	3.606878	2.751304
H	0.879759	1.612728	0.253176	H	-1.086601	3.457329	0.621192
C	2.526453	-0.863628	-0.260971	H	-2.028055	2.292835	1.549105
H	2.852927	0.133215	-0.550010	C	-1.915277	4.650865	2.975487
C	-2.525328	-0.862873	-0.262805	H	-0.779171	2.933779	3.619078
H	-2.851348	0.134031	-0.552151	H	0.152572	4.102795	2.695406
N	11.156101	0.578014	-0.634778	H	-1.733690	5.230745	3.887764
N	-11.155583	0.578880	-0.634367	H	-1.965703	5.356608	2.136736
C	-3.012565	-3.136180	0.402326	H	-2.901462	4.179803	3.071302
C	-1.655726	-3.431169	0.483135	C	-0.045500	1.731721	-1.291629
C	1.655572	-3.431522	0.484724	C	1.046336	2.779425	-1.485952
C	3.012570	-3.136934	0.404893	H	-1.022077	2.234510	-1.325471
H	-3.740924	-3.911780	0.631668	H	-0.036341	1.042357	-2.147206
H	-1.332473	-4.428564	0.773114	C	0.827259	3.606789	-2.751256
H	1.331847	-4.428772	0.774702	H	1.086562	3.457308	-0.621138
H	3.740528	-3.912705	0.634905	H	2.028049	2.292808	-1.549009
C	-4.921566	-1.636136	-0.020502	C	1.915230	4.650783	-2.975475
H	-5.520068	-2.510898	0.234239	H	0.779146	2.933661	-3.619009
H	-4.954583	0.386540	-0.597272	H	-0.152610	4.102694	-2.695371
C	4.922318	-1.637588	-0.017609	H	1.733635	5.230628	-3.887773
H	5.520593	-2.511900	0.239208	H	1.965645	5.356559	-2.136750
H	4.955510	0.383579	-0.599337	H	2.901421	4.179733	-3.071272
C	11.632747	1.900215	-0.995982	C	12.038854	1.095664	0.615643
C	11.646753	2.922263	0.143355	C	13.383328	1.364287	-0.055534

H	11.033004	2.283957	-1.832841	H	12.109486	1.339674	1.692003
H	12.649659	1.785610	-1.389105	H	11.318222	1.790606	0.177646
C	12.067665	4.309794	-0.330785	C	13.823574	2.814729	0.126967
H	10.651119	2.973329	0.604173	H	14.162077	0.704756	0.349886
H	12.332037	2.576455	0.929125	H	13.299507	1.133911	-1.126384
C	12.114099	5.333565	0.797832	C	15.167392	3.109031	-0.529661
H	13.055238	4.247963	-0.810833	H	13.057586	3.483649	-0.290332
H	11.372076	4.654364	-1.109714	H	13.880975	3.046378	1.200111
H	12.414869	6.321392	0.430669	H	15.461054	4.155180	-0.387610
H	11.132426	5.439522	1.275559	H	15.960754	2.479994	-0.107358
H	12.829050	5.034283	1.574079	H	15.130901	2.916495	-1.608916
C	12.138005	-0.437025	-0.300347	C	12.437438	-1.340938	0.795099
C	12.414210	-0.611287	1.195079	C	13.121768	-2.042919	-0.378025
H	13.071163	-0.169245	-0.809536	H	11.880831	-2.076488	1.390949
H	11.828386	-1.396983	-0.735856	H	13.202956	-0.933228	1.469670
C	13.380972	-1.758183	1.473039	C	14.018319	-3.189395	0.079579
H	12.824917	0.324665	1.597582	H	12.360423	-2.420879	-1.073840
H	11.468823	-0.785625	1.726256	H	13.713754	-1.312623	-0.944689
C	13.689689	-1.927974	2.956222	C	14.717817	-3.893641	-1.077500
H	12.958616	-2.693193	1.077180	H	14.770973	-2.804633	0.783218
H	14.316820	-1.589412	0.920527	H	13.419253	-3.918354	0.644356
H	14.381824	-2.759999	3.128696	H	15.354051	-4.712383	-0.722644
H	14.147586	-1.021637	3.371137	H	13.989996	-4.317292	-1.780392
H	12.776300	-2.129139	3.529262	H	15.352521	-3.196932	-1.638814
C	-11.632916	1.900924	-0.995162	C	-12.038753	1.095661	-0.615651
C	-11.651397	2.921635	0.145293	C	-13.383309	1.364289	0.055356
H	-12.648626	1.785546	-1.391207	H	-12.109231	1.339745	-1.692007
H	-11.031364	2.286376	-1.829905	H	-11.318154	1.790550	-0.177508
C	-12.073893	4.308874	-0.328321	C	-13.823489	2.814752	-0.127139
H	-12.337869	2.573701	0.929089	H	-14.162021	0.704799	-0.350199
H	-10.656919	2.974016	0.608466	H	-13.299643	1.133866	1.126208
C	-12.125603	5.331211	0.801361	C	-15.167383	3.109066	0.529328
H	-11.376936	4.655832	-1.104960	H	-13.057534	3.483631	0.290286
H	-13.060029	4.245531	-0.811121	H	-13.880745	3.046448	-1.200281
H	-12.427419	6.318835	0.434514	H	-15.460988	4.155234	0.387296
H	-12.842093	5.029521	1.575255	H	-15.960712	2.480081	0.106886
H	-11.145495	5.438667	1.281960	H	-15.131042	2.916470	1.608577
C	-12.137116	-0.437071	-0.301507	C	-12.437397	-1.340934	-0.795211
C	-12.412244	-0.614531	1.193746	C	-13.121841	-2.042921	0.377839
H	-11.827750	-1.396104	-0.739274	H	-11.880752	-2.076484	-1.391021
H	-13.070643	-0.168269	-0.809443	H	-13.202846	-0.933201	-1.469847
C	-13.378927	-1.761905	1.470023	C	-14.018528	-3.189249	-0.079870
H	-11.466485	-0.790118	1.723848	H	-12.360559	-2.421036	1.073640
H	-12.822523	0.320610	1.598548	H	-13.713742	-1.312593	0.944550
C	-13.686501	-1.934800	2.953094	C	-14.718064	-3.893549	1.077154
H	-14.315192	-1.591850	0.918613	H	-14.771163	-2.804327	-0.783441
H	-12.957003	-2.696132	1.071860	H	-13.419557	-3.918209	-0.644747
H	-14.378593	-2.767113	3.124354	H	-15.354405	-4.712177	0.722230
H	-12.772687	-2.137275	3.524991	H	-13.990264	-4.317364	1.779970
H	-14.143972	-1.029293	3.370285	H	-15.352666	-3.196831	1.638572

7. Molecule **CN-PV** (PBE0/6-31+G(d)/Toluene)

CN-PV(*a*)				**CN-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	-4.890015	0.054614	-0.275555	C	-9.662198	-1.916342	0.107290
C	-3.474329	0.043927	-0.628052	C	-8.302084	-2.185065	0.111696
C	-2.527638	0.033830	0.415412	C	-7.348708	-1.168615	-0.080526
C	-1.172906	0.016263	0.131560	C	-7.819293	0.142025	-0.289433
C	-0.729233	0.011110	-1.201887	C	-9.174210	0.424700	-0.295737
C	0.000117	0.000742	1.097228	C	-10.109414	-0.603893	-0.095680
C	1.172978	-0.014403	0.131362	H	-10.381148	-2.715647	0.260147
C	0.729092	-0.008326	-1.202011	H	-7.963235	-3.205967	0.270996
C	2.527745	-0.032422	0.414984	H	-7.118883	0.954629	-0.456788
C	3.474266	-0.042161	-0.628627	H	-9.519922	1.441097	-0.459077
C	4.889944	-0.053813	-0.276228	C	-5.934161	-1.525955	-0.055801
C	5.940429	0.003908	-1.121575	C	-4.890821	-0.672373	-0.121423
C	7.351827	-0.007769	-0.751434	C	-3.472405	-1.013773	-0.098603
C	7.811281	-0.170085	0.569727	C	-1.175172	-0.226814	-0.031135
C	9.163758	-0.167909	0.863646	C	-0.726806	-1.559083	-0.064785
C	10.107675	-0.005078	-0.163564	C	0.000044	0.745827	-0.022231
C	9.671626	0.152911	-1.485873	C	1.175876	-0.225557	-0.053942
H	10.397351	0.277395	-2.283976	C	0.728343	-1.558300	-0.076286
C	8.313763	0.149235	-1.765846	C	3.473689	-1.013367	-0.014409
H	9.500901	-0.294959	1.888060	C	4.891326	-0.671785	0.034543
H	7.104099	-0.305787	1.382344	C	5.935433	-1.526913	0.043661
H	7.983540	0.273334	-2.794425	C	7.349085	-1.169517	0.095807
C	-0.016120	-1.254731	2.000389	C	8.303758	-2.202718	0.079888
C	-0.034880	-2.598342	1.278780	C	9.663666	-1.936924	0.126428
H	-0.893187	-1.184033	2.660274	C	10.109267	-0.609984	0.191725
H	0.863535	-1.207701	2.658949	C	9.172595	0.436448	0.209832
C	-0.049747	-3.780764	2.244407	H	9.516958	1.465034	0.261501
H	-0.915974	-2.655139	0.624534	C	7.818000	0.156602	0.162868
C	-0.069290	-5.128186	1.531625	H	10.383691	-2.749666	0.112693
H	0.830771	-3.725604	2.900853	H	7.966067	-3.235214	0.029579
H	-0.926595	-3.701462	2.903271	H	7.116458	0.985053	0.180378
H	-0.079492	-5.959981	2.245308	C	-2.535950	0.038499	-0.069685
H	-0.956577	-5.224915	0.893765	H	-2.904140	1.061870	-0.086168
H	0.812905	-5.249095	0.890819	C	2.536523	0.038662	-0.004273
C	0.016509	1.256017	2.000706	H	2.904070	1.060645	0.055758
C	0.035320	2.599780	1.279387	C	2.999679	-2.339535	-0.063431
C	0.050021	3.782019	2.245234	C	1.641276	-2.616397	-0.086998
C	0.069597	5.129558	1.532679	C	-1.638972	-2.617233	-0.101047
H	-0.830588	3.726706	2.901547	C	-2.997644	-2.340457	-0.111419
H	0.926782	3.702633	2.904204	H	-3.700959	-3.167516	-0.147708
H	0.079647	5.961240	2.246494	H	-1.294971	-3.648357	-0.131837
H	0.956972	5.226429	0.894963	H	1.298018	-3.648053	-0.105850
H	-0.812511	5.250515	0.891761	H	3.703268	-3.167035	-0.072807
H	0.842951	-2.678728	0.622597	H	5.744127	-2.598338	0.009288
H	0.916484	2.656736	0.625250	H	5.090459	0.399037	0.067367
H	-0.842440	2.680273	0.623124	H	-5.091401	0.396750	-0.186684
H	0.893612	1.185098	2.660521	H	-5.741144	-2.593504	0.039230
H	-0.863120	1.208889	2.659296	C	0.091014	1.573600	1.285372

H	2.878302	-0.036375	1.446441	C	-0.993806	2.615763	1.539312
H	-2.878035	0.037013	1.446928	H	1.067408	2.077396	1.293866
C	3.008778	-0.041111	-1.959517	H	0.113373	0.867272	2.126700
C	1.652392	-0.023857	-2.251339	C	-0.729246	3.417496	2.812526
H	1.321600	-0.025619	-3.287236	H	-1.065247	3.310946	0.690578
H	3.719630	-0.059256	-2.780716	H	-1.972688	2.127292	1.628718
C	-1.652703	0.027232	-2.251056	C	-1.808439	4.455995	3.096014
C	-3.009036	0.043962	-1.959015	H	-0.649912	2.727298	3.664366
H	-3.720005	0.062488	-2.780096	H	0.247787	3.915123	2.730994
H	-1.322070	0.029781	-3.287002	H	-1.593250	5.017874	4.011999
H	5.081521	-0.105566	0.795212	H	-1.889218	5.178038	2.273806
H	5.756654	0.077787	-2.192419	H	-2.790547	3.982828	3.219237
C	11.503773	-0.003926	0.139152	C	-0.091910	1.627312	-1.294048
N	12.640237	-0.002760	0.386388	C	0.993828	2.677724	-1.506396
C	-5.940427	-0.003466	-1.120979	H	-1.067693	2.132146	-1.279525
C	-7.351878	0.006962	-0.751067	H	-0.116750	0.956667	-2.164014
C	-7.811689	0.167322	0.570203	C	0.724698	3.535957	-2.741224
H	-7.104743	0.302324	1.383137	H	1.070795	3.334121	-0.627853
C	-8.313526	-0.149395	-1.765858	H	1.971228	2.191764	-1.622173
C	-9.164222	0.163950	0.863849	C	1.806499	4.581604	-2.985760
H	-9.501644	0.289444	1.888364	H	0.636815	2.884408	-3.622174
C	-9.671443	-0.154261	-1.486165	H	-0.249592	4.033524	-2.631262
H	-10.396933	-0.278228	-2.284566	H	1.587607	5.184603	-3.874308
H	-7.983022	-0.272046	-2.794520	H	1.896075	5.265942	-2.132799
C	-10.107846	0.001804	-0.163742	H	2.785632	4.110327	-3.136802
C	-11.504008	-0.000661	0.138715	C	-11.508019	-0.313104	-0.103532
N	-12.640514	-0.002902	0.385746	C	11.507466	-0.321506	0.240468
H	-5.081609	0.105846	0.795911	N	12.645712	-0.085854	0.280019
H	-5.756501	-0.076683	-2.191840	N	-12.646566	-0.075634	-0.109607

8. Molecule **SO_2CF_3-PV** (PBE0/6-31+G(d)/toluene)

SO_2CF_3-PV(*a*)				**SO_2CF_3-PV(*b*)**			
atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
C	9.664227	-0.634402	-1.477840	C	9.64976	-0.62377	-1.56953
C	8.307584	-0.611395	-1.765220	C	8.29343	-0.54189	-1.84733
C	7.346872	-0.363569	-0.766574	C	7.33519	-0.44917	-0.82022
C	7.799737	-0.130494	0.547257	C	7.78971	-0.44539	0.51345
C	9.149976	-0.150190	0.853065	C	9.13977	-0.52598	0.81001
C	10.074290	-0.402860	-0.164806	C	10.06206	-0.61319	-0.23695
H	10.396376	-0.840823	-2.252603	H	10.37978	-0.70683	-2.36891
H	7.977799	-0.797543	-2.784219	H	7.96202	-0.55495	-2.88265
H	7.090764	0.069470	1.344393	H	7.08181	-0.3837	1.33397
H	9.491655	0.017950	1.869834	H	9.48256	-0.53417	1.84024
C	5.937908	-0.366069	-1.145077	C	5.92723	-0.36719	-1.19269
C	4.886708	-0.235218	-0.308378	C	4.87995	-0.28267	-0.34531
C	3.472420	-0.241368	-0.663642	C	3.4672	-0.19979	-0.69737
C	2.524873	-0.187044	0.377604	C	2.52335	-0.1435	0.34718
C	1.170635	-0.202998	0.092038	C	1.17068	-0.06656	0.06398
C	0.729581	-0.269301	-1.240786	C	0.72791	-0.04183	-1.26956
C	-0.003671	-0.157959	1.054808	C	-0.00024	0.00046	1.02962
C	-1.174556	-0.213232	0.088388	C	-1.17092	0.0675	0.0637

C	-0.728845	-0.275708	-1.243050	C	-0.72783	0.04271	-1.26974
C	-2.529790	-0.209444	0.369691	C	-2.52366	0.14451	0.34657
C	-3.473800	-0.270232	-0.674485	C	-3.46726	0.20076	-0.6982
C	-4.889020	-0.271491	-0.323259	C	-4.88009	0.28372	-0.34646
C	-5.938729	-0.369178	-1.166256	C	-5.92729	0.36681	-1.19408
C	-7.348571	-0.372430	-0.791415	C	-7.3353	0.44897	-0.82187
C	-7.802929	-0.210080	0.532556	C	-7.78975	0.44983	0.51184
C	-9.154364	-0.228871	0.832826	C	-9.13986	0.53019	0.80816
C	-10.078432	-0.409799	-0.200488	C	-10.0623	0.6126	-0.23905
C	-9.666713	-0.572714	-1.523237	C	-9.65008	0.6187	-1.57168
H	-10.398731	-0.725470	-2.310464	H	-10.38023	0.6981	-2.37133
C	-8.308879	-0.551803	-1.804969	C	-8.29368	0.53709	-1.84925
H	-9.497178	-0.115832	1.856796	H	-9.48259	0.54202	1.83837
H	-7.094292	-0.068555	1.342437	H	-7.08173	0.39214	1.33254
H	-7.977873	-0.684965	-2.831845	H	-7.96234	0.5467	-2.88464
S	11.793472	-0.427670	0.219552	S	11.78125	-0.71551	0.13458
O	12.518240	-1.180359	-0.798881	O	12.49947	-1.2944	-0.99601
O	11.978951	-0.672603	1.646175	O	11.96571	-1.19508	1.50037
S	-11.799224	-0.434180	0.176775	O	-11.96643	1.19894	1.49629
C	-0.010185	1.143963	1.890311	O	-12.50029	1.28909	-1.0004
C	-0.015502	2.447807	1.098949	S	-11.78157	0.71476	0.13219
H	0.867883	1.123541	2.552255	C	-12.3193	-1.08067	0.18243
H	-0.888746	1.115619	2.551296	F	-13.61602	-1.13003	0.46196
C	-0.021588	3.679453	2.001016	F	-11.64132	-1.73808	1.12091
H	0.864250	2.485958	0.441436	F	-12.10048	-1.66036	-0.99585
C	-0.027465	4.987622	1.218456	C	0.07138	1.25393	1.93305
H	-0.900350	3.642622	2.661068	C	0.14533	2.59592	1.21196
H	0.856995	3.650883	2.661738	H	0.94621	1.14539	2.59069
H	-0.031966	5.855701	1.887515	H	-0.80775	1.24369	2.59384
H	0.857306	5.067103	0.574743	C	0.21521	3.77582	2.17829
H	-0.912295	5.058662	0.573838	H	1.02533	2.61524	0.55401
C	0.000680	-1.363574	2.023627	C	0.28873	5.12171	1.46619
C	0.007071	-2.743972	1.375050	H	-0.66375	3.75765	2.8388
C	0.011452	-3.872963	2.402778	H	1.09092	3.65855	2.83295
C	0.018270	-5.256816	1.763525	H	0.3379	5.95164	2.18036
H	0.889186	-3.766342	3.056569	H	1.17615	5.18111	0.82396
H	-0.868220	-3.774376	3.055234	H	-0.59073	5.28074	0.82999
H	0.021166	-6.048909	2.521009	C	-0.07208	-1.25307	1.93295
H	-0.865348	-5.404073	1.130254	C	-0.14584	-2.59503	1.21178
H	0.904329	-5.396060	1.131859	C	-0.21596	-3.77497	2.17803
H	-0.894720	2.478108	0.440384	C	-0.28929	-5.12082	1.46586
H	-0.871588	-2.851651	0.723891	H	0.66283	-3.75683	2.83878
H	0.887485	-2.843960	0.724978	H	-1.09184	-3.65774	2.83248
H	-0.878101	-1.272786	2.678660	H	-0.33865	-5.95079	2.17997
H	0.878249	-1.265447	2.679226	H	-1.17654	-5.1802	0.82338
C	12.318630	1.354278	-0.034751	H	0.59034	-5.27983	0.82989
F	11.636014	2.156241	0.779912	H	-0.73088	2.71492	0.5595
F	13.615075	1.459006	0.231142	H	-1.02567	-2.61433	0.55359
F	12.096210	1.724822	-1.293903	H	0.73055	-2.71399	0.55953
H	2.873782	-0.138071	1.408348	H	-0.94709	-1.14458	2.59037
H	-2.882158	-0.163058	1.399371	H	0.80687	-1.24286	2.59396
C	3.010299	-0.300285	-1.994312	C	12.32046	1.07963	0.17857
C	1.654502	-0.314886	-2.287974	F	11.64326	1.74078	1.11499
C	-1.650145	-0.331793	-2.292964	F	13.61729	1.1289	0.4576
C	-3.006941	-0.328137	-2.003595	F	12.10179	1.65548	-1.00161

H	-3.716597	-0.368692	-2.824926
H	-1.317821	-0.377503	-3.327261
H	1.325713	-0.359641	-3.323429
H	3.722977	-0.330156	-2.813512
H	-5.755914	-0.465547	-2.235193
H	-5.081266	-0.191489	0.746133
H	5.076457	-0.123950	0.758672
H	5.756572	-0.503316	-2.209817
O	-12.530324	-1.112931	-0.888098
O	-11.993386	-0.763807	1.584985
C	-12.299828	1.366767	0.030675
F	-11.612323	2.107866	0.897115
F	-12.064774	1.811466	-1.201906
F	-13.596442	1.471943	0.295349

H	2.87371	-0.16245	1.37845
H	-2.87427	0.16352	1.37775
C	3.00287	-0.17345	-2.02851
C	1.64883	-0.09554	-2.31981
C	-1.6485	0.09643	-2.3202
C	-3.00261	0.1744	-2.02924
H	-3.71195	0.21392	-2.85088
H	-1.3171	0.07775	-3.35566
H	1.31767	-0.07683	-3.35534
H	3.71242	-0.21283	-2.84998
H	-5.74353	0.37737	-2.26708
H	-5.07239	0.27741	0.72598
H	5.07211	-0.27519	0.72714
H	5.74355	-0.37954	-2.26569

SO_2CF_3-PV(*c*)

atom	*x*	*y*	*z*
C	9.660576	-0.741452	-1.164986
C	8.330513	-0.658221	-1.549087
C	7.300351	-0.487340	-0.605003
C	7.654529	-0.401284	0.756031
C	8.976922	-0.482331	1.158255
C	9.972555	-0.651547	0.191632
H	10.446571	-0.886234	-1.899855
H	8.077410	-0.733427	-2.603693
H	6.889039	-0.271870	1.514528
H	9.241981	-0.427156	2.209757
C	5.925299	-0.414019	-1.086564
C	4.816800	-0.297271	-0.325304
C	3.435422	-0.225675	-0.787706
C	1.088588	-0.048649	-0.211678
C	0.748838	-0.093543	-1.574560
C	-0.151662	0.066946	0.656256
C	-1.247364	0.081668	-0.395761
C	-0.701318	-0.006449	-1.692371
C	-3.474325	0.175051	-1.329074
C	-4.925597	0.267967	-1.221284
C	-5.651620	0.370588	-0.087940
C	-7.104664	0.461945	0.002110
C	-7.690609	0.551372	1.278983
C	-9.064967	0.639768	1.442662
C	-9.875699	0.640542	0.307494
C	-9.330057	0.558443	-0.977010
H	-9.979155	0.576733	-1.847260
C	-7.955750	0.470682	-1.120871
H	-9.506027	0.719152	2.431599
H	-7.050467	0.555790	2.157675
H	-7.542342	0.414203	-2.122877
S	11.657063	-0.754819	0.697531
O	12.446709	-1.411118	-0.339235
O	11.730273	-1.153250	2.099417
O	-11.946377	1.313581	1.803882
O	-12.226429	1.249588	-0.734591

S	-11.623836	0.750250	0.497032
C	-12.159205	-1.043582	0.600953
F	-13.478044	-1.087762	0.744978
F	-11.582353	-1.636794	1.643839
F	-11.815746	-1.691499	-0.510306
C	-0.173532	1.360971	1.514608
C	-0.259430	2.715808	0.806827
H	0.712426	1.347176	2.165871
H	-1.038926	1.272866	2.186655
C	1.008923	3.209013	0.111554
H	-1.090863	2.708297	0.088319
C	0.863621	4.639805	-0.395847
H	1.852506	3.151954	0.814904
H	1.266558	2.551893	-0.726620
H	1.777755	4.983597	-0.893293
H	0.041511	4.720829	-1.118049
H	0.649806	5.333888	0.426857
C	-0.270501	-1.128117	1.640358
C	-0.082670	-2.549180	1.102983
C	-1.221170	-3.121640	0.259639
C	-1.010494	-4.598129	-0.058688
H	-2.171314	-2.993036	0.798427
H	-1.323980	-2.560675	-0.676061
H	-1.830840	-4.998505	-0.665321
H	-0.078359	-4.752425	-0.616678
H	-0.949475	-5.198067	0.858189
H	-0.534874	3.457585	1.571067
H	0.857446	-2.611440	0.537315
H	0.052845	-3.204205	1.976380
H	-1.247332	-1.055053	2.140282
H	0.480017	-0.960201	2.425761
C	12.224353	1.032054	0.675478
F	11.490364	1.758317	1.516009
F	13.496976	1.080321	1.049798
F	12.106467	1.537752	-0.550300
C	2.415328	-0.120584	0.177394
H	2.685892	-0.093454	1.232146
C	-2.613109	0.177888	-0.212866
H	-3.021746	0.250570	0.792375
C	3.074595	-0.256414	-2.150848
C	1.747073	-0.194013	-2.548011
C	-1.536215	-0.012030	-2.808883
C	-2.910059	0.076223	-2.616017
H	-3.571757	0.071469	-3.479608
H	-1.130191	-0.085440	-3.814820
H	1.495656	-0.221724	-3.605615
H	3.844829	-0.332408	-2.912840
H	-5.138286	0.388459	0.872064
H	-5.445681	0.249248	-2.178407
H	5.823663	-0.467259	-2.169177
H	4.926060	-0.253049	0.757925

9. Molecule **SO_2CF_3-PE** (PBE0/6-31+G(d)/toluene)

SO_2CF_3-PE(*a*)				**SO_2CF_3-PE(*b*)**			
atom	x	y	z	atom	x	y	z
C	9.729681	0.513987	-1.135278	C	9.711556	-0.589679	-1.213016
C	8.369352	0.577500	-1.394382	C	8.353111	-0.504563	-1.475692
C	7.435518	0.399821	-0.355142	C	7.424010	-0.444074	-0.418995
C	7.895145	0.161512	0.954615	C	7.886121	-0.473985	0.911045
C	9.253864	0.095930	1.221592	C	9.243038	-0.558540	1.181849
C	10.156986	0.270591	0.171376	C	10.141805	-0.613543	0.114933
H	10.454925	0.662071	-1.929532	H	10.432048	-0.649183	-2.023006
H	8.015809	0.770182	-2.402360	H	7.996931	-0.489768	-2.500896
H	7.176216	0.033153	1.757655	H	7.170180	-0.435738	1.726026
H	9.615004	-0.076217	2.230883	H	9.605140	-0.594102	2.204768
C	6.043587	0.464118	-0.625074	C	6.033921	-0.360303	-0.692761
C	4.849571	0.515579	-0.858266	C	4.841598	-0.288934	-0.929246
C	3.456391	0.571075	-1.130348	C	3.450665	-0.206345	-1.205702
C	2.523712	0.413388	-0.084835	C	2.520170	-0.150367	-0.147886
C	1.171628	0.464159	-0.370429	C	1.170339	-0.069743	-0.437316
C	0.729136	0.670721	-1.690444	C	0.728300	-0.043546	-1.773268
C	-0.001001	0.321128	0.584255	C	-0.000058	0.000271	0.528364
C	-1.173272	0.465225	-0.370703	C	-1.170423	0.070416	-0.437344
C	-0.730290	0.671468	-1.690610	C	-0.728342	0.044363	-1.773288
C	-2.525477	0.415847	-0.085433	C	-2.520260	0.151012	-0.147940
C	-3.457699	0.574576	-1.131195	C	-3.450729	0.207087	-1.205772
C	-4.850980	0.520477	-0.859598	C	-4.841676	0.289591	-0.929363
C	-6.045138	0.470073	-0.626979	C	-6.034012	0.360719	-0.692873
C	-7.437139	0.405961	-0.357666	C	-7.424105	0.444261	-0.419066
C	-7.897347	0.176069	0.953356	C	-7.886184	0.474375	0.910982
C	-9.256120	0.109316	1.219632	C	-9.243116	0.558653	1.181804
C	-10.158654	0.274296	0.167367	C	-10.141924	0.613176	0.114899
C	-9.730775	0.509913	-1.140504	C	-9.711705	0.589118	-1.213056
H	-10.455709	0.650587	-1.936382	H	-10.432231	0.648258	-2.023042
C	-8.370381	0.574891	-1.398854	C	-8.353250	0.504279	-1.475748
H	-9.617762	-0.056694	2.229775	H	-9.605200	0.594345	2.204725
H	-7.178818	0.054852	1.757859	H	-7.170209	0.436497	1.725952
H	-8.016353	0.761421	-2.407805	H	-7.997096	0.489334	-2.500958
S	11.888853	0.182828	0.505464	S	11.871541	-0.721057	0.454856
O	12.629124	0.875849	-0.543117	O	12.567967	-1.273629	-0.701636
O	12.130724	0.428905	1.922791	O	12.077482	-1.231884	1.805587
O	-12.135301	0.438139	1.915028	O	-12.077707	1.231201	1.805549
O	-12.632409	0.863644	-0.554940	O	-12.568214	1.272773	-0.701674
S	-11.890515	0.182083	0.499979	S	-11.871682	0.720370	0.454832
C	-12.272796	-1.638556	0.263147	C	-12.403410	-1.076342	0.528909
C	12.279447	-1.634188	0.255011	F	-13.704809	-1.124015	0.783236
F	-13.566987	-1.832591	0.482571	F	-11.741463	-1.711784	1.492976
F	-11.565087	-2.371675	1.119318	F	-12.158353	-1.676176	-0.633678
F	-11.974436	-2.013071	-0.978690	C	0.074923	1.253963	1.431473
F	11.985835	-1.999951	-0.990549	C	0.153615	2.595753	0.710451
F	11.572626	-2.377110	1.103439	H	0.948858	1.142237	2.089519

F	13.573895	-1.824520	0.476241
C	-0.000609	1.431672	1.661584
C	0.000122	2.867096	1.145788
H	0.877781	1.275329	2.304350
H	-0.879264	1.276166	2.304188
C	0.000981	3.893271	2.276279
H	0.879779	3.032163	0.508106
C	0.001553	5.331476	1.770945
H	-0.877751	3.729535	2.916654
H	0.879907	3.728645	2.916155
H	0.002231	6.048033	2.600221
H	0.886378	5.533598	1.154743
H	-0.883530	5.534513	1.155411
C	-0.001651	-1.053280	1.293638
C	-0.001720	-2.276697	0.382742
C	-0.002023	-3.587839	1.164862
C	-0.002239	-4.816050	0.261927
H	0.876776	-3.617651	1.825080
H	-0.880875	-3.617315	1.825029
H	-0.002441	-5.743444	0.845967
H	-0.887143	-4.829887	-0.386341
H	0.882691	-4.830232	-0.386296
H	-0.879635	3.033209	0.508522
H	-0.881306	-2.249137	-0.275500
H	0.878049	-2.249436	-0.275260
H	-0.879896	-1.090610	1.954409
H	0.876116	-1.091117	1.955021
H	-2.885753	0.255815	0.927914
H	2.883546	0.252985	0.928610
C	-3.003640	0.783495	-2.449450
C	-1.645388	0.832384	-2.732771
C	1.644665	0.830546	-2.732396
C	3.002798	0.780459	-2.448710
H	3.732554	0.901174	-3.243997
H	1.310249	0.991110	-3.754231
H	-1.310573	0.993069	-3.754458
H	-3.733118	0.905050	-3.244866
H	-0.804705	1.245976	2.091387
C	0.225923	3.774865	1.677601
H	1.034595	2.613266	0.053736
C	0.304464	5.120742	0.966103
H	-0.653978	3.758905	2.336808
H	1.100547	3.654385	2.333028
H	0.355334	5.950014	1.680859
H	1.192940	5.177780	0.325131
H	-0.573808	5.282898	0.329067
C	-0.075060	-1.253529	1.431312
C	-0.153529	-2.595233	0.710103
C	-0.225758	-3.774494	1.677075
C	-0.304099	-5.120275	0.965374
H	0.654103	-3.758528	2.336337
H	-1.100435	-3.654213	2.332468
H	-0.354907	-5.949659	1.680005
H	-1.192533	-5.177325	0.324345
H	0.574227	-5.282231	0.328361
H	-0.721620	2.718152	0.057265
H	-1.034460	-2.612761	0.053321
H	0.721768	-2.717430	0.056961
H	-0.949091	-1.141968	2.089258
H	0.804480	-1.245552	2.091343
C	12.403627	1.075549	0.528812
F	11.742604	1.710939	1.493540
F	13.705250	1.122957	0.782033
F	12.157685	1.675627	-0.633474
H	2.879860	-0.171723	0.877985
H	-2.879975	0.172244	0.877926
C	2.997353	-0.180402	-2.540435
C	1.641493	-0.099526	-2.827882
C	-1.641503	0.100476	-2.827919
C	-2.997381	0.181295	-2.540497
H	-3.725519	0.225761	-3.345144
H	-1.306588	0.082278	-3.861975
H	1.306603	-0.081204	-3.861945
H	3.725511	-0.224810	-3.345067

SO_2CF_3-PE(*c*)

atom	*x*	*y*	*z*
C	9.709617	-0.614903	-1.091238
C	8.351272	-0.527053	-1.353484
C	7.422250	-0.470492	-0.296510
C	7.884303	-0.507420	1.033366
C	9.241134	-0.594748	1.303756
C	10.139838	-0.645555	0.236582
H	10.430039	-0.671269	-1.901513
H	7.995108	-0.506901	-2.378602
H	7.168377	-0.472320	1.848501
H	9.603224	-0.635573	2.326484
C	6.032296	-0.383279	-0.569902
C	4.840111	-0.308928	-0.806086
C	3.449382	-0.221195	-1.082290

C	1.170107	-0.072974	-0.313878
C	0.727721	-0.049635	-1.649995
C	0.000010	0.000036	0.650176
C	-1.170104	0.072950	-0.313868
C	-0.727739	0.049418	-1.649990
C	-3.449391	0.221058	-1.082262
C	-4.840113	0.308845	-0.806053
C	-6.032303	0.383219	-0.569907
C	-7.422280	0.470464	-0.296637
C	-7.884397	0.508260	1.033194
C	-9.241246	0.595631	1.303464
C	-10.139912	0.645596	0.236220
C	-9.709633	0.614073	-1.091562
H	-10.430025	0.669798	-1.901907
C	-8.351264	0.526197	-1.353690
H	-9.603386	0.637127	2.326147
H	-7.168499	0.473804	1.848381
H	-7.995054	0.505380	-2.378780
S	11.869478	-0.756030	0.575971
O	12.565423	-1.304416	-0.582803
O	12.075073	-1.272598	1.924570
O	-12.075298	1.273548	1.923698
O	-12.565528	1.303656	-0.583717
S	-11.869580	0.756110	0.575451
C	-12.402996	-1.039754	0.657951
F	-13.704467	-1.085008	0.912396
F	-11.741720	-1.671288	1.625033
F	-12.158432	-1.645263	-0.501795
C	0.052498	1.246152	1.575743
C	-0.084464	2.637473	0.952207
H	0.988440	1.196242	2.150626
H	-0.755832	1.121301	2.309917
C	1.118692	3.161372	0.169112
H	-0.979319	2.674227	0.315381
C	0.945144	4.621062	-0.236988
H	2.024826	3.055257	0.783196
H	1.286294	2.554280	-0.727702
H	1.811743	4.986176	-0.799915
H	0.058244	4.752136	-0.869630
H	0.821816	5.266284	0.642029
C	-0.052466	-1.246013	1.575832
C	0.084534	-2.637373	0.952391
C	-1.118595	-3.161346	0.169302
C	-0.944995	-4.621050	-0.236726
H	-2.024742	-3.055227	0.783365
H	-1.286198	-2.554301	-0.727544
H	-1.811573	-4.986217	-0.799651
H	-0.058080	-4.752126	-0.869346
H	-0.821663	-5.266227	0.642323
H	-0.280185	3.337177	1.778103
H	0.979403	-2.674153	0.315587
H	0.280249	-3.337019	1.778338
H	-0.988417	-1.196081	2.150698
H	0.755853	-1.121096	2.310005
C	12.403081	1.039830	0.657302

F	11.741920	1.672047	1.624017
F	13.704570	1.085115	0.911652
F	12.158518	1.644628	-0.502815
C	2.519437	-0.164357	-0.024786
H	2.878972	-0.188692	1.001032
C	-2.519426	0.164375	-0.024766
H	-2.878941	0.188869	1.001054
C	2.996400	-0.189301	-2.417261
C	1.640658	-0.106312	-2.704783
C	-1.640693	0.105933	-2.704770
C	-2.996433	0.188959	-2.417234
H	-3.724727	0.232406	-3.221815
H	-1.305843	0.084676	-3.738808
H	1.305788	-0.085213	-3.738818
H	3.724680	-0.232873	-3.221847

10. Molecule **NH_2-PE** (PBE0/6-31+G(d)/toluene)

NH_2-PE			
atom	*x*	*y*	*z*
C	9.753236	0.023022	0.952519
C	8.394673	0.012862	1.223634
C	7.445573	0.010665	0.184984
C	7.920919	0.019641	-1.139392
C	9.278964	0.029826	-1.413344
C	10.222280	0.032100	-0.372019
H	10.466441	0.019863	1.774189
H	8.052582	0.007055	2.254951
H	7.207727	0.020163	-1.959191
H	9.620235	0.030627	-2.446446
C	3.465135	-0.015839	0.988994
C	1.173312	-0.019391	0.229946
C	0.729651	-0.024475	1.565299
C	-0.001123	-0.017224	-0.734762
C	-1.174737	-0.018341	0.231017
C	-0.729903	-0.023957	1.565997
C	-3.465905	-0.014837	0.992240
C	-7.446310	0.014656	0.187517
C	-8.397454	0.033761	1.224328
C	-9.755559	0.047254	0.950665
C	-10.222164	0.041861	-0.374735
C	-9.276859	0.022445	-1.414212
H	-9.616102	0.022809	-2.447982
C	-7.919356	0.009154	-1.137703
H	-10.470317	0.067046	1.770768
H	-8.057319	0.037045	2.256304
H	-7.204693	-0.006829	-1.956082
C	-0.002175	-1.271263	-1.640204
C	-0.003694	-2.616330	-0.921177
H	0.876789	-1.212121	-2.298831
H	-0.880940	-1.210359	-2.298933

C	-0.004825	-3.797047	-1.888963
H	0.875830	-2.686951	-0.266239
C	-0.007059	-5.145967	-1.178707
H	-0.883333	-3.727339	-2.546831
H	0.874603	-3.729814	-2.545825
H	-0.007606	-5.976921	-1.893690
H	0.877216	-5.256725	-0.538901
H	-0.892511	-5.254430	-0.540109
C	-0.000348	1.238815	-1.636373
C	0.003780	2.581247	-0.912537
C	0.007200	3.765529	-1.875897
C	0.012269	5.111728	-1.160543
H	0.885553	3.696482	-2.534043
H	-0.872376	3.702463	-2.532984
H	0.014917	5.945384	-1.872366
H	-0.871944	5.222036	-0.520579
H	0.897763	5.215758	-0.521266
H	-0.883594	-2.684949	-0.266494
H	-0.875521	2.650958	-0.257164
H	0.883869	2.645712	-0.257655
H	-0.880370	1.182549	-2.293827
H	0.877349	1.179030	-2.296624
C	2.525170	-0.015335	-0.062955
H	2.880942	-0.010944	-1.090715
C	-2.526870	-0.014016	-0.060556
H	-2.883571	-0.008950	-1.087978
N	11.578510	-0.018610	-0.644007
N	-11.576685	0.115876	-0.649356
C	-3.008297	-0.021648	2.326243
C	-1.649672	-0.026247	2.616242
C	1.650388	-0.027413	2.614683
C	3.008767	-0.023156	2.323455
H	3.739201	-0.025073	3.127575
H	1.319083	-0.031862	3.650509
H	-1.317463	-0.030994	3.651779
H	-3.737982	-0.022430	3.131069
H	-12.197023	-0.197514	0.084848
H	-11.865190	-0.214823	-1.560129
H	11.862713	0.315634	-1.554837
H	12.191860	0.307524	0.090522
C	-4.859587	-0.006987	0.712539
C	-6.054138	0.002250	0.469690
C	4.858454	-0.007839	0.707420
C	6.052998	0.000500	0.464459

11. Molecule **CN-PE** (PBE0/6-31+G(d)/toluene)

CN-PE			
atom	*x*	*y*	*z*

C	4.851766	-0.007121	0.742854
C	3.458427	-0.009749	1.021361
C	2.524887	-0.007141	-0.035340
C	1.172668	-0.008073	0.254545
C	0.729680	-0.011709	1.590368
C	-0.000077	-0.005010	-0.711185
C	-1.172792	-0.006141	0.254580
C	-0.729740	-0.010491	1.590380
C	-2.525032	-0.003467	-0.035278
C	-3.458568	-0.005198	1.021431
C	-4.851965	-0.002153	0.743070
C	-7.437258	0.004365	0.219802
C	-7.895570	0.009632	-1.111187
C	-9.252884	0.013591	-1.388651
C	-10.181607	0.012327	-0.337265
C	-9.736364	0.006967	0.993049
H	-10.458284	0.005992	1.804022
C	-8.378217	0.003020	1.266777
H	-9.601691	0.017714	-2.416766
H	-7.174858	0.010670	-1.923079
H	-8.030798	-0.001049	2.295259
C	-0.001187	-1.259253	-1.616592
C	-0.002472	-2.604486	-0.897656
H	0.877282	-1.199379	-2.275429
H	-0.879486	-1.197748	-2.275506
C	-0.003688	-3.784557	-1.866306
H	0.877187	-2.676112	-0.242876
C	-0.005076	-5.133679	-1.156547
H	-0.882483	-3.714662	-2.523534
H	0.875231	-3.716470	-2.523556
H	-0.005950	-5.963680	-1.872331
H	0.879738	-5.245047	-0.517648
H	-0.890104	-5.243205	-0.517626
C	0.001041	1.252728	-1.611594
C	0.002778	2.595099	-0.887351
C	0.004352	3.778944	-1.851384
C	0.006596	5.125290	-1.136391
H	0.882968	3.711159	-2.509078
H	-0.874738	3.713852	-2.508709
H	0.007699	5.958066	-1.848943
H	-0.877990	5.234614	-0.496825
H	0.891852	5.231883	-0.497288
H	-0.882202	-2.674390	-0.242788
H	-0.876808	2.664422	-0.232228
H	0.882579	2.662126	-0.232281
H	-0.877560	1.195630	-2.270493
H	0.879173	1.193682	-2.270952
H	-2.884880	0.000010	-1.061341
H	2.884746	-0.003993	-1.061400
C	-3.004138	-0.009752	2.355964
C	-1.645785	-0.012391	2.644006
H	-1.311380	-0.015676	3.678457
H	-3.733725	-0.011057	3.160587
C	1.645730	-0.015069	2.643994
C	3.004080	-0.014053	2.355926

H	3.733695	-0.016271	3.160521
H	1.311339	-0.018176	3.678445
C	-11.582433	0.016577	-0.622168
N	-12.721706	0.020069	-0.854242
C	7.436965	0.001035	0.219421
C	7.895492	0.004582	-1.111490
H	7.174938	0.003099	-1.923520
C	8.377691	0.002903	1.266589
C	9.252852	0.009983	-1.388700
H	9.601858	0.012706	-2.416752
C	9.735864	0.008325	0.993117
H	10.457637	0.009810	1.804221
H	8.030049	0.000146	2.295005
C	10.181354	0.011952	-0.337119
C	11.582233	0.017679	-0.621713
N	12.721560	0.022371	-0.853498
C	-6.045638	0.000695	0.501801
C	6.045369	-0.003822	0.501314

12. Molecule **NBu_2-PV-SO_2CF_3** (PBE0/6-31+G(d)/toluene)

NBu_2-PV-SO_2CF_3			
atom	*x*	*y*	*z*
C	-8.879105	-0.382349	0.955044
C	-7.518994	-0.525737	1.158259
C	-6.568727	0.106629	0.335843
C	-7.081568	0.885035	-0.711993
C	-8.443388	1.039568	-0.931992
C	-9.396373	0.423108	-0.090618
H	-9.547773	-0.906680	1.628088
H	-7.192029	-1.154223	1.982978
H	-6.388445	1.383049	-1.388341
H	-8.756135	1.641286	-1.776826
C	-5.128221	-0.011272	0.504885
C	-3.022888	-0.823953	1.612468
C	-0.737424	-0.331674	0.984778
C	-0.260988	-1.127860	2.044354
C	0.414881	0.271962	0.197497
C	1.611916	-0.287873	0.949141
C	1.195845	-1.101182	2.023661
C	3.925987	-0.697998	1.516179
C	5.972729	0.147812	0.324840
C	7.411353	0.295561	0.142460
C	8.366902	-0.198075	1.053659
C	9.723030	-0.034468	0.828853
C	10.146265	0.637130	-0.322252
C	9.230185	1.148267	-1.242345
H	9.576700	1.681370	-2.122456
C	7.875965	0.974272	-1.000764
H	10.452780	-0.406906	1.541437

H	8.049336	-0.708404	1.957491
H	7.155198	1.373265	-1.710152
C	0.387366	1.817540	0.233946
C	0.392724	2.454046	1.619943
H	-0.505251	2.151388	-0.315196
H	1.251660	2.185250	-0.338845
C	0.366035	3.979375	1.563378
H	-0.474579	2.098114	2.193009
C	0.369753	4.624235	2.944769
H	1.232636	4.337655	0.988815
H	-0.524803	4.306998	1.008089
H	0.350172	5.718139	2.877760
H	-0.503608	4.309833	3.529440
H	1.265711	4.340468	3.510747
C	0.402011	-0.184308	-1.279813
C	0.421651	-1.691187	-1.514180
C	0.407879	-2.053168	-2.997152
C	0.426484	-3.557984	-3.240726
H	-0.483767	-1.616212	-3.469710
H	1.273640	-1.590485	-3.493060
H	0.415909	-3.792028	-4.311538
H	1.323676	-4.017284	-2.807478
H	-0.445610	-4.042461	-2.784466
H	1.284368	2.128429	2.173780
H	1.313833	-2.127437	-1.043603
H	-0.445069	-2.152480	-1.020982
H	1.266482	0.273927	-1.782798
H	-0.490614	0.245783	-1.757301
C	-2.093887	-0.179324	0.768444
H	-2.444558	0.439648	-0.054486
C	2.954114	-0.086344	0.696042
H	3.260265	0.547260	-0.133500
N	-10.756870	0.612372	-0.262067
C	3.491388	-1.503897	2.586301
C	2.141732	-1.711752	2.846980
C	-1.161645	-1.773978	2.891017
C	-2.524231	-1.615953	2.667498
H	4.236784	-1.976308	3.222966
H	1.838495	-2.340405	3.680704
H	-0.813646	-2.393279	3.714747
H	-3.233473	-2.116569	3.323606
C	5.359688	-0.537563	1.314309
H	5.973824	-1.045435	2.057449
H	5.367401	0.641620	-0.433568
C	-4.468857	-0.714247	1.452108
H	-5.046499	-1.269931	2.190543
H	-4.547248	0.543788	-0.232238
S	11.869437	0.845351	-0.614399
O	12.604724	0.727091	0.640750
C	12.332229	-0.689658	-1.586110
O	12.087284	1.952201	-1.540329
C	-11.195937	1.370111	-1.428659
C	-12.675350	1.732525	-1.455262
H	-10.938280	0.836812	-2.361540
H	-10.632091	2.310478	-1.441139

C	-12.986132	2.688823	-2.605325
H	-13.297987	0.834883	-1.568301
H	-12.959131	2.204284	-0.504182
C	-14.466704	3.039849	-2.693445
H	-12.397141	3.608488	-2.483240
H	-12.659078	2.237784	-3.552948
H	-14.664141	3.730068	-3.521222
H	-15.077911	2.143276	-2.854322
H	-14.815824	3.518263	-1.770146
C	-11.689083	-0.331049	0.335612
C	-11.773491	-1.679290	-0.380687
H	-12.676692	0.136755	0.358906
H	-11.422670	-0.477642	1.387474
C	-12.750742	-2.637123	0.293540
H	-12.079221	-1.514562	-1.424268
H	-10.774032	-2.134064	-0.419449
C	-12.851810	-3.981223	-0.418649
H	-12.440540	-2.797410	1.336269
H	-13.745699	-2.170962	0.340199
H	-13.557410	-4.650531	0.086566
H	-13.193744	-3.855565	-1.453375
H	-11.878114	-4.485151	-0.450967
F	11.640476	-0.742548	-2.722436
F	12.074212	-1.782948	-0.871255
F	13.629712	-0.643911	-1.864413