Electronic Supplementary Information

Quantitative Topological Descriptor for Linear Co-oligomers Fusion

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1. Computational details

On the basis of our previous findings,[1] the ground state geometries of neutral and single charged states (cation, anion) were fully optimised at Density Functional Theory (DFT) level, using B3LYP[2] hybrid functional coupled with 6-311++G**[3,4] basis set including GD3BJ[5] empirical dispersion. The presence of imaginary frequencies was checked in harmonic approximation for all optimised geometries and minima of the potential energy surface were found to be "genuine". The enthalpies and Gibbs energies of formations were calculated for all investigated compounds alongside with the frequency calculations. Ionisation potential (I) of investigated compounds was evaluated as the difference between single-point energy (SPE) of optimised cationic form and neutral forms. Electron affinity of investigated compounds was evaluated as the difference between SPE of optimised anionic and neutral forms.

To explore vertical excited states, nature and energies of first 10 singlet and triplet states were evaluated at Time-Dependent Density Functional Theory (TD-TDF) within the framework of Tamm-Dancoff approximation (TDA)[6] employing PBE0[7]/6-311++G** level of theory. According to our previous investigation,[1] this level of theory was shown to give best agreement with experimental data for 5Oa and 5Sa systems. The geometries of first singlet excited state S_1 were optimised at TD(A)-DFT PBE0/6-311++G** level of theory.

The reorganisation energies for hole (λ_h) and electron (λ_e) transfer were calculated from potential energy surfaces (equation 1 and 2)[8] at DFT B3LYP[GD3BJ]/6-311++G** level of theory and refined integration grid (*vide postea*).

$$\lambda_h = \left(E^{+}_{neutral(eq)} - E^{0}_{neutral(eq)}\right) + \left(E^{0}_{cation(eq)} - E^{+}_{cation(eq)}\right) \quad (1)$$

$$\lambda_e = \left(E^{-}_{neutral(eq)} - E^{0}_{neutral(eq)}\right) + \left(E^{0}_{anion(eq)} - E^{-}_{anion(eq)}\right) \quad (2)$$

Exciton couplings were evaluated for model, "sandwich-like" co-facial π-dimers as the half of T_1 vertical excitation energy calculated at TD(A)-DFT PBE0/6-311++G** level of theory. Distance between mass centres of the molecules in the dimer was set to 3.5, 4.0 and 4.5 Å.

The first polarisability (both static and frequency dependent) of investigated compounds was evaluated using long-range corrected CAM-B3LYP[9] coupled with 6-31+G*[10] basis set (this level of theory was previously shown to have the best agreement with experimental data).[11] The dynamic properties have been evaluated at the working frequencies of common laser sources, *viz.* ω = 0.6502 eV (λ = 1907 nm), 0.6561 eV (λ = 1890 nm), 0.9051 eV (λ = 1370 nm), 1.1698 eV (λ = 1064 nm), 1.3626 eV (λ = 910 nm), and 1.4940 eV (λ = 830 nm).

Integration grid for the SPE calculations required for reorganisation energy evaluation was set to 150 radial shells and 974 angular points. In other cases, integration grid was set as 99 radial shells and 590 angular points. Convergence criteria of Self-Consistent Field were set to 10^{-10} for root mean square (RMS) change in density matrix and 10^{-8} for maximum change in density matrix. Convergence criteria for optimisations of neutral, cationic and anionic ground states in the gas phase were set to 2×10^{-6} a.u. for maximum force, 1×10^{-6} a.u. for RMS force, 6×10^{-6} a.u. for maximum displacement and 4×10^{-6} a.u. for RMS displacement; for optimisation of S_1 excited state, convergence criteria for optimisations were set to 4.5×10^{-4} a.u. for maximum force, 3.0×10^{-4} a.u. for RMS force, 1.8×10^{-3} a.u. for maximum displacement and 1.2×10^{-3} a.u. for RMS displacement.

All calculations were performed using GAUSSIAN G09.D01 package.[12]

2. General description and summary of computational results

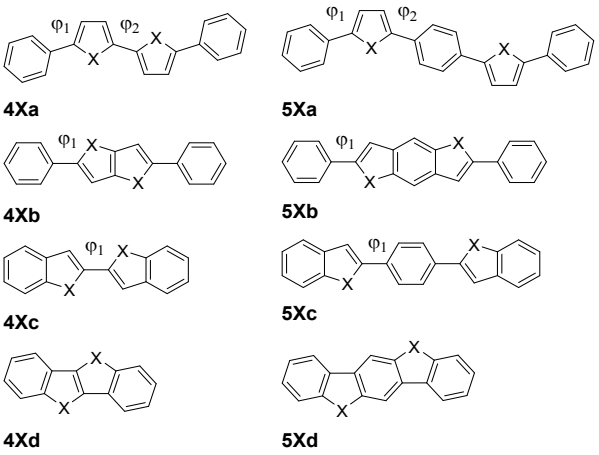

Chart S1. Chemical formula of investigated compounds and dihedral angles designation.

The geometries of studied molecules (Chart S1) were optimised at DFT level of theory and found to be planar for all furan-containing systems while thiophene-containing ones have distorted geometry for both annulated and non-annulated compounds (Table S1; see part 5 for optimised geometries coordinates). This difference is ascribed to the more efficient conjugation and hence higher torsional rigidity of furan compounds as compared with their thiophene analogues.[1] Bond length alternation of investigated compounds was found to be lower for furan-containing compounds, which is also a sign of more efficient conjugation (Table S1). The geometries of single charged cations of investigated compounds were also optimised at DFT level of theory and found to be planar for all systems except thiophene/phenylenes which remain to be slightly distorted.

Table S1. Values of dihedral angles (φ_1; φ_2) and bond length alternation (BLA) of investigated compounds optimised geometries in neutral and charged states.

	φ_1/φ_2 (degs)			BLA (Å)		
	neutral	cationic	anionic	neutral	cationic	anionic
4Oa	0/0	0/0	0/0	0.060	0.038	0.023
4Ob	0	0	0	0.054	0.027	0.020
4Oc	0	0	0	0.047	0.02	0.015
4Sa	27/18	11/2	0/0	0.072	0.058	0.049
4Sb	28	0	0	0.069	0.040	0.025
4Sc	13	0	0	0.050	0.038	0.018
5Oa	0/0	0/0	0/0	0.064	0.038	0.041
5Ob	0	0	0	0.063	0.038	0.038
5Oc	0	0	0	0.046	0.026	0.028
5Sa	27/24	0/0	16/1	0.076	0.043	0.043
5Sb	27	14	0	0.074	0.042	0.040
5Sc	26	0	0	0.057	0.044	0.038

Single point energies of investigated compounds in all forms (Table S2) were calculated alongside with the geometry optimisation and found to decrease upon the increase of annulation degree due to lower amount of electrons in annulated compounds.

Table S2. Single-point energy of investigated systems (hartree).

	Furans (X=O)			Thiophenes (X=S)		
	neutral	cation	anion	neutral	cation	anion
4Xa	-921.299	-921.062	-921.325	-1567.269	-1567.029	-1567.307
4Xb	-843.831	-843.588	-843.856	-1489.824	-1489.576	-1489.855
4Xc	-766.418	-766.158	-766.441	-1412.394	-1412.111	-1412.423
4Xd	-688.954	-688.686	-688.962	-1334.953	-1334.686	-1334.965
5Xa	-1152.441	-1152.210	-1152.477	-1798.407	-1798.173	-1798.451
5Xb	-997.558	-997.315	-997.589	-1643.530	-1643.284	-1643.566
5Xc	-997.560	-997.312	-997.597	-1643.532	-1643.282	-1643.572
5Xd	-842.683	-842.412	-842.704	-1488.660	-1488.396	-1488.683

Electron gaps between frontier molecular orbitals (HOMO, LUMO, E_g) were found to increase (Table S3) which is a consequence of a fewer number of π-electrons in annulated compounds. Energies of the HOMO of investigated compounds were found to decrease with the increase of annulation degree. No monotonic trend is observed in the case of LUMO energy.

Table S3. Energy of frontier molecular orbitals (HOMO, LUMO) and electron gap (E_g) of investigated compounds (eV)

	Furans (X=O)			Thiophenes (X=S)		
	HOMO	LUMO	E_g	HOMO	LUMO	E_g
4Xa	-5.241	-1.816	3.425	-5.436	-2.028	3.408
4Xb	-5.323	-1.826	3.497	-5.594	-1.832	3.761
4Xc	-5.774	-1.847	3.927	-5.848	-1.984	3.864
4Xd	-5.872	-1.542	4.331	-5.863	-1.634	4.229
5Xa	-5.224	-1.986	3.238	-5.466	-2.057	3.409
5Xb	-5.460	-1.931	3.529	-5.552	-1.940	3.612
5Xc	-5.632	-2.097	3.535	-5.776	-2.043	3.733
5Xd	-6.058	-1.842	4.216	-5.835	-1.828	4.006

The increase is observed for ionisation potential (I_p) of 4O, 5O, 4S compounds and for electron affinity (E_a) of 4O, 4S compounds (Table S4), however no monotonic trends are observed for other compounds.

Table S4. Ionisation potential (I_p) and electron affinity (E_a) of investigated compounds (eV)

	Furans (X=O)		Thiophenes (X=S)	
	I_p	E_a	I_p	E_a
4Xa	6.448	-0.703	6.538	-1.051
4Xb	6.605	-0.679	6.759	-0.836
4Xc	7.090	-0.604	7.694	-0.802
4Xd	7.305	-0.193	7.266	-0.348
5Xa	6.280	-0.972	6.407	-1.196
5Xb	6.630	-0.846	6.698	-0.979
5Xc	6.760	-0.997	6.808	-1.082
5Xd	7.360	-0.586	7.185	-0.624

The enthalpy (ΔH_f) and Gibbs energy (ΔG_f) of formation were evaluated for all investigated compounds at T = 298.15 K and p = 1.00 atm (Tables S5) and found to decrease with the increase of the annulation degree.

Table S5. Enthalpy and Gibbs free energy of formation of all investigated compounds calculated at T = 298.15 K and p = 1.00 atm ($kJ \cdot mol^{-1}$)

	Furans (X=O)		Thiophenes (X=S)	
	ΔH_f	ΔG_f	ΔH_f	ΔG_f
4Xa	-13912	-12866	-14399	-13329
4Xb	-12474	-11540	-13023	-12064
4Xc	-11182	-10357	-11684	-10839
4Xd	-9754	-9041	-10314	-9580
5Xa	-18031	-16675	-18508	-17125
5Xb	-15295	-14158	-15788	-14629
5Xc	-15300	-14164	-15793	-14634
5Xd	-12575	-11660	-13082	-12148

Optical properties investigation of the furan/ and thiophene/phenylenes showed that $S_0 \rightarrow S_{1v}$ transition retains to be the brightest one for all non-annulated and partially annulated compounds. The nature of this transition retains to be mainly HOMO → LUMO without presence of intermolecular charge transfer for all investigated compounds. On the other hand, $S_0 \rightarrow S_{1v}$ transition is mostly dark for fully-annulated compound whilst $S_0 \rightarrow S_{2v}$ is the brightest one. Monotonic increase was observed for both absorption and emission energies (Table S6). Stokes' shifts did not show any dependency from annulation degree.

Table S6. Absorption energy (first bright absorption band) and emission energy ($S_1 \rightarrow S_0$) of investigated compounds (eV).

	Furans (X=O)		Thiophenes (X=S)	
	Absorption	Emission	Absorption	Emission
4Xa	3.399	3.136	3.355	2.902
4Xb	3.584	3.363	3.720	3.254
4Xc	4.022	3.748	3.754	3.528
4Xd	4.369	4.067	4.383	3.758
5Xa	3.169	2.903	3.290	2.771
5Xb	3.549	3.271	3.533	3.147
5Xc	3.527	3.240	3.645	3.180
5Xd	4.134	3.818	4.143	3.430

First static and dynamic (evaluated at the working frequencies of common laser sources) molecular electric polarisabilities (Table S7) were found to increase with the increase of the annulation degree as well as with the increase of excitation frequency.

Table S7. First static and dynamic (evaluated for λ = 1907 nm, 1370 nm, 1064 nm, 910 nm and 830 nm) molecular electric polarisabilities of investigated compounds (10^{-24} cm^3).

	4-ring systems						**5-ring systems**					
	Furan			Thiophene			Furan			Thiophene		
	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm
a	41.2	41.7	42.3	46.0	46.5	47.1	55.7	56.4	57.3	59.7	60.3	61.2
b	37.4	37.9	38.4	40.5	40.9	41.3	45.9	46.4	47.0	50.2	50.7	51.2
c	31.6	31.9	31.9	36.2	36.5	36.9	46.0	46.6	47.2	49.7	50.2	50.7
d	25.7	25.9	26.1	30.0	30.2	30.4	33.8	34.1	34.3	38.5	38.8	39.1
	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm
a	42.9	43.6	44.2	47.7	48.5	49.0	58.3	59.5	60.4	62.1	63.1	63.9
b	39.0	39.6	40.1	41.8	42.3	42.7	47.7	48.4	49.0	51.8	52.6	53.1
c	32.6	33.0	33.3	37.3	37.7	38.1	47.9	48.6	49.2	51.3	52.0	52.5
d	26.3	26.5	26.7	30.7	30.9	31.1	34.7	35.0	35.3	39.5	39.8	40.0

Exciton coupling of all investigated compounds in model co-facial π-stacking dimers was found to decrease with the increase of the distance between mass-centres of molecules (Table S8).

Table S8. Exciton couplings in the model π-stacking dimer (evaluated for distance between mass-centres equal to 3.5 Å; 4.0 Å and 4.5 Å) of investigated compounds (meV).

	4-rings						5-rings					
	Furan			Thiophene			Furan			Thiophene		
	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å
a	732	863	899	592	739	788	697	851	886	626	778	809
b	769	904	933	732	879	924	802	948	983	807	891	945
c	892	1029	1066	917	1008	1072	798	967	977	780	910	953
d	1087	1224	1256	1041	1201	1251	1204	1341	1382	1123	1308	1361

Reorganisation energy was evaluated for both hole (λ_h) and electron (λ_e) transport for all investigated compounds (Table S9). Both 4 and 5-ringed furan derivatives were found to have higher hole reorganisation energy for fully annulated compounds 4Od and 5Od as compared with their non-annulated analogues 4Oa and 5Oa. On the other hand thiophene-containing compounds demonstrate 1.5 and 3 times lower hole reorganisation energy for 4Sd and 4Sa; 5Sd and 5Sa respectively. Electron reorganisation energy was found to be generally higher for thiophene-containing compounds as compared with their furan analogues, however monotonic trend was found only for 5-ringed thiophene compounds.

Table S9. Reorganisation energies for hole (λ_h) and electron (λ_e) transfer of investigated compounds (meV)

	Furans (X=O)		Thiophenes (X=S)	
	λ_h	λ_e	λ_h	λ_e
4Xa	259	269	343	411
4Xb	246	297	336	450
4Xc	262	315	273	321
4Xd	300	267	225	167
5Xa	217	226	347	416
5Xb	258	229	271	367
5Xc	255	269	311	386
5Xd	243	197	118	224

3. Summary of correlations with F-index

3.1 Values of Adj-R^2 by linear regressions

Legend for Tables S10 - S23

The following tables report values of Adj-R^2 for linear regressions of different molecular properties as a function of the F-index variants. Values are classified by the quality of regression: **bold** (excellent: adj-R^2 > 0.9500), underlined (good: 0.9000 ≤ adj-R^2 < 0.9500), *Italics* (decent: 0.8500 ≤ adj-R^2 < 0.9000), plain (poor adj-R^2 < 0.8500).

Table S10. Single-point energy in neutral state.

SPE (neutral form)				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8049	0.7001	*0.8800*	*0.8715*
4S	0.8048	0.7000	*0.8800*	*0.8714*
5O	0.8216	0.8012	0.7712	0.7995
5S	0.8216	0.8012	0.7712	0.7995

Table S11. Single-point energy in cationic state.

SPE (cationic form)				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8049	0.7001	*0.8800*	*0.8715*
4S	0.8047	0.6999	*0.8799*	*0.8714*
5O	0.8216	0.8012	0.7712	0.7995
5S	0.8216	0.8012	0.7712	0.7995

Table S12. Single-point energy in anionic state.

SPE (anionic form)				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8049	0.7002	*0.8800*	*0.8715*
4S	0.8049	0.7001	*0.8800*	*0.8715*
5O	0.8216	0.8012	0.7712	0.7995
5S	0.8216	0.8012	0.7712	0.7995

Table S13. Energy of HOMO.

HOMO				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.5915	0.3944	0.7384	0.6688
4S	0.4510	0.2930	0.5932	0.5507
5O	0.8288	0.7739	*0.8582*	*0.8753*
5S	0.3159	0.2342	0.3852	0.4079

Table S14. Energy of LUMO.

	LUMO			
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.7677	0.8251	0.6492	0.6846
4S	0.6336	0.8109	0.4880	0.5945
5O	0.3599	0.4377	0.2763	0.2594
5S	*0.8542*	0.9039	0.7495	0.7558

Table S15. HOMO-LUMO gap.

	HOMO-LUMO gap			
	F_{00}	F_{01}	F_{10}	F_{11}
4O	*0.8800*	0.7294	**0.9580**	0.9142
4S	0.8444	0.8220	*0.8580*	*0.8930*
5O	**0.9786**	**0.9546**	**0.9760**	**0.9851**
5S	0.7843	0.7309	0.8003	0.8225

Table S16. Ionisation potential.

	Ionisation potential			
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.7157	0.5433	0.8377	0.7862
4S	-0.0807	-0.2360	0.0798	0.0110
5O	*0.8878*	0.8455	*0.8957*	0.9131
5S	0.8230	0.7785	0.8223	0.8453

Table S17. Electron affinity.

	Electron affinity			
	F_{00}	F_{01}	F_{10}	F_{11}
4O	**0.9653**	0.9414	0.9170	0.9274
4S	**0.9663**	**0.9805**	0.9237	**0.9671**
5O	*0.8883*	0.9259	0.8301	0.8235
5S	**0.9873**	**0.9958**	0.9383	0.9460

Table S18. Enthalpy of formation.

	Enthalpy of formation			
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8112	0.7089	*0.8812*	*0.8745*
4S	0.8059	0.7123	*0.8800*	*0.8782*
5O	0.8205	0.8128	0.7687	0.7809
5S	0.8207	0.7999	0.7803	0.8050

Table S19. Gibbs' free energy of formation.

Gibbs' free energy of formation				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8045	0.7052	*0.8845*	*0.8720*
4S	0.8086	0.7025	*0.8853*	*0.8740*
5O	0.8250	0.8012	0.7756	0.7968
5S	0.8210	0.8032	0.7712	0.7912

Table S20. Absorption and emission energies.

Transition energy (absorption)				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8332	0.6882	0.9241	*0.8887*
4S	0.9396	**0.9601**	0.9004	0.9495
5O	0.9476	0.9293	0.9175	0.9348
5S	0.9020	0.8577	0.9209	0.9349

Transition energy (emission)				
	F_{00}	F_{01}	F_{10}	F_{11}
4O	0.8239	0.6909	0.9115	*0.8846*
4S	0.7115	0.6150	0.7931	0.7909
5O	0.9474	0.9312	0.9135	0.9312
5S	0.6618	0.6358	0.6070	0.6418

Table S21. First electric polarisability.

	4-ring systems						5-ring systems					
	Furan			Thiophene			Furan			Thiophene		
	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm	Static	1907 nm	1370 nm
F_{00}	*0.8578*	*0.8598*	*0.8563*	*0.8529*	*0.8506*	0.8481	*0.8882*	*0.8903*	*0.8856*	*0.8632*	*0.8657*	*0.8753*
F_{01}	0.7350	0.7373	0.7338	0.7708	0.7685	0.7642	*0.8681*	*0.8704*	*0.8712*	0.8378	0.8405	0.8485
F_{10}	0.9341	0.9355	0.9310	0.9067	0.9048	0.9048	0.8476	0.8476	0.8462	0.8281	0.8281	0.8257
F_{11}	0.9126	0.9136	0.9123	0.9100	0.9098	0.9107	*0.8711*	*0.8699*	*0.8680*	*0.8529*	*0.8537*	*0.8542*
	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm	1064 nm	910 nm	830 nm
F_{00}	*0.8582*	*0.8563*	*0.8526*	*0.8501*	*0.8512*	*0.8521*	*0.8882*	*0.8875*	*0.8854*	*0.8712*	*0.8732*	*0.8729*
F_{01}	0.7348	0.7317	0.7328	0.7624	0.7662	0.7646	*0.8732*	*0.8724*	*0.8737*	0.8495	0.8475	0.8480
F_{10}	0.9327	0.9304	0.9300	0.9023	0.9031	0.9049	0.8485	0.8474	0.8482	0.8241	0.8256	0.8230
F_{11}	0.9136	0.9128	0.9137	0.9112	0.9109	0.9112	*0.8682*	*0.8680*	*0.8696*	*0.8553*	*0.8542*	*0.8555*

Table S22. Exciton couplings (at 3.5, 4.0 and 4.5 Å of distance).

	4-ring systems						5-ring systems					
	Furan			Thiophene			Furan			Thiophene		
	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å	3.5 Å	4.0 Å	4.5 Å
F_{00}	0.9454	0.9468	0.9474	*0.8941*	*0.8959*	*0.8931*	0.9432	0.9412	0.9414	0.9007	0.9016	0.9032
F_{01}	0.8287	0.8293	0.8270	0.8130	0.8131	0.8123	0.9079	0.9082	0.9076	0.8218	0.8213	0.8219
F_{10}	**0.9899**	**0.9912**	**0.9910**	0.9430	0.9426	0.9433	**0.9854**	**0.9882**	**0.9878**	0.9341	0.9354	0.9351
F_{11}	**0.9601**	**0.9641**	**0.9637**	0.9432	0.9438	0.9434	**0.9822**	**0.9819**	**0.9809**	**0.9957**	**0.9975**	**0.9931**

Table S23. Reorganisation energies for hole (λ_h) and electron (λ_e) transfer.

	4-ring systems				**5-ring systems**			
	Furan		Thiophene		Furan		Thiophene	
	λ_h	λ_e	λ_h	λ_e	λ_h	λ_e	λ_h	λ_e
F_{00}	0.7792	-0.3689	0.8372	*0.8511*	-0.3922	0.1737	**0.9928**	**0.9956**
F_{01}	0.6898	-0.3171	0.6707	0.7012	-0.3906	0.2334	**0.9998**	**0.9894**
F_{10}	0.7604	-0.4313	0.9304	0.9001	-0.4379	0.1418	0.9562	**0.9875**
F_{11}	0.7242	-0.4230	*0.8773*	0.8436	-0.4209	0.1143	0.9594	**0.9870**

3.2 Intercepts and slopes obtained by linear regressions

The following tables report values of intercepts (Tables S24, S26, S28, S30) and slopes (Tables S25, S27, S29, S31) with respective errors, obtained for different molecular properties of different compounds as a function of the F-index variants by means of the least squares linear regression. Values are classified by the quality of regression: **bold** (excellent: adj-R^2 > 0.9500), underlined (good: 0.9000 ≤ adj-R^2 < 0.9500), *Italics* (decent: 0.8500 ≤ adj-R^2 < 0.9000), plain (poor adj-R^2 < 0.8500).

Table S24. Intercepts (with errors) for 4O-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	-880 ± 30	-880 ± 40	*-890 ± 20*	*-890 ± 30*
$E_{SPE}(+)$	-880 ± 30	-880 ± 40	*-890 ± 20*	*-890 ± 30*
$E_{SPE}(-)$	-880 ± 30	-880 ± 40	*-890 ± 20*	*-890 ± 30*
I_p	6.6 ± 0.2	6.5 ± 0.2	6.5 ± 0.1	6.5 ± 0.1
E_a	**-0.75 ± 0.03**	-0.75 ± 0.04	-0.75 ± 0.05	-0.76 ± 0.05
E_{HOMO}	-5.3 ± 0.1	-5.3 ± 0.2	-5.3 ± 0.1	-5.3 ± 0.1
E_{LUMO}	-1.87 ± 0.05	-1.88 ± 0.04	-1.87 ± 0.06	-1.86 ± 0.06
E_g	*3.4 ± 0.1*	3.5 ± 0.2	**3.43 ± 0.06**	3.42 ± 0.09
ΔH_f	-16000 ± 700	-16000 ± 900	*-16000 ± 600*	*-16200 ± 600*
ΔG_f	-15000 ± 700	-15000 ± 800	*-15000 ± 500*	*-15000 ± 600*
E_{Abs}	3.5 ± 0.1	3.5 ± 0.2	3.46 ± 0.09	*3.5 ± 0.1*
E_{Em}	3.2 ± 0.1	3.3 ± 0.2	3.22 ± 0.09	*3.2 ± 0.1*
α(0;0)	40 ± 2	39 ± 2	40 ± 1	40 ± 1
α(-1907 nm; 1907 nm)	40 ± 1	39 ± 2	40 ± 1	40 ± 2
α(-1370 nm; 1370 nm)	40 ± 2	40 ± 1	39 ± 2	40 ± 1
α(-1064 nm; 1064 nm)	40 ± 1	39 ± 1	40 ± 2	39 ± 1
α(-910 nm; 910 nm)	39 ± 2	40 ± 2	40 ± 1	39 ± 2
α(-830 nm; 830 nm)	40 ± 2	40 ± 1	39 ± 2	40 ± 1
λ_h	248 ± 8	248 ± 9	248 ± 8	247 ±9
λ_e	290 ± 20	290 ± 18	290 ± 20	290 ± 20
V_{exc} (3.5 Å)	830 ± 30	720 ± 30	**860 ± 10**	**850 ± 30**
V_{exc} (4.0 Å)	820 ± 30	730 ± 40	**870 ± 10**	**840 ± 30**
V_{exc} (4.5 Å)	830 ± 30	720 ± 40	**870 ± 10**	**850 ± 30**

Table S25. Slopes (with errors) for 4O-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	35 ± 9	50 ± 18	*31 ± 6*	*40 ± 10*
$E_{SPE}(+)$	35 ± 9	50 ± 18	*31 ± 6*	*40 ± 10*
$E_{SPE}(-)$	35 ± 9	50 ± 18	*31 ± 6*	*40 ± 10*
I_p	0.14 ± 0.05	0.19 ± 0.09	0.12 ± 0.03	0.17 ± 0.05
E_a	**0.09 ± 0.01**	0.13 ± 0.02	0.07 ± 0.01	0.11 ± 0.02
E_{HOMO}	-0.10 ± 0.04	-0.14 ± 0.08	-0.09 ± 0.03	-0.12 ± 0.05
E_{LUMO}	0.05 ± 0.02	0.08 ± 0.02	0.04 ± 0.01	0.06 ± 0.02
E_g	*0.15 ± 0.03*	0.22 ± 0.07	**0.13 ± 0.02**	0.19 ± 0.03
ΔH_f	800 ± 200	1200 ± 400	*800 ± 200*	*1000 ± 200*
ΔG_f	800 ± 200	1100 ± 400	*700 ± 100*	*1000 ± 200*
E_{Abs}	0.16 ± 0.04	0.22 ± 0.08	0.14 ± 0.02	*0.19 ± 0.04*
E_{Em}	0.15 ± 0.04	0.21 ± 0.08	0.13 ± 0.02	*0.18 ± 0.04*
α(0;0)	-2.4 ± 0.5	-3 ± 1	-2.1 ± 0.3	-3.1 ± 0.5
α(-1907 nm; 1907 nm)	-2.2 ± 0.3	-2 ± 1	-2.0 ± 0.2	3.2 ± 0.6
α(-1370 nm; 1370 nm)	-2.5 ± 0.4	-3 ± 1	-2.0 ± 0.3	-3.0 ± 0.4
α(-1064 nm; 1064 nm)	-2.4 ± 0.4	-3 ± 1	-2.1 ± 0.2	-3.1 ± 0.4
α(-910 nm; 910 nm)	-2.3 ± 0.3	-3 ± 1	-2.2 ± 0.2	-3.0 ± 0.5
α(-830 nm; 830 nm)	-2.2 ± 0.4	-2 ± 1	-2.1 ± 0.2	-3.2 ± 0.4
λ_h	8 ± 2	11 ± 4	7 ± 2	10 ± 3
λ_e	-3 ± 6	-5 ± 9	2 ± 5	-2 ± 7
V_{exc} (3.5 Å)	61 ± 8	90 ± 20	**54 ± 2**	**74 ± 7**
V_{exc} (4.0 Å)	58 ± 7	90 ± 20	**55 ± 3**	**76 ± 6**
V_{exc} (4.5 Å)	60 ± 10	100 ± 30	**52 ± 3**	**73 ± 8**

Table S26. Intercepts (with errors) for 4S-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	-1530 ± 30	-1530 ± 40	*-1530 ± 40*	*-1530 ± 40*
$E_{SPE}(+)$	-1530 ± 30	-1530 ± 40	*-1530 ± 40*	*-1530 ± 40*
$E_{SPE}(-)$	-1530 ± 30	-1530 ± 40	*-1530 ± 40*	*-1530 ± 40*
I_p	6.8 ± 0.4	6.9 ± 0.4	6.7 ± 0.4	6.8 ± 0.4
E_a	**-1.01 ± 0.04**	**-1.01 ± 0.03**	-1.01 ± 0.06	**-1.03 ± 0.04**
E_{HOMO}	-5.5 ± 0.1	-5.6 ± 0.1	-5.5 ± 0.1	-5.5 ± 0.1
E_{LUMO}	-2.00 ± 0.07	-2.00 ± 0.05	-2.00 ± 0.09	2.00 ± 0.08
E_g	3.5 ± 0.1	3.5 ± 0.1	*3.5 ± 0.1*	*3.51 ± 0.08*
ΔH_f	-16000 ± 700	-16000 ± 900	*-16000 ± 600*	*-16000 ± 600*
ΔG_f	-15000 ± 700	-15000 ± 800	*-15000 ± 500*	*-15600 ± 600*
E_{Abs}	3.44 ± 0.07	**3.43 ± 0.06**	3.4 ± 0.1	3.41 ± 0.07
E_{Em}	3.1 ± 0.1	3.1 ± 0.2	3.0 ± 0.1	3.0 ± 0.1
α(0;0)	44 ± 2	43 ± 2	44 ± 1	42 ± 3
α(-1907 nm; 1907 nm)	43 ± 2	44 ± 2	42 ± 3	43 ± 2
α(-1370 nm; 1370 nm)	43 ± 2	43 ± 2	44 ± 1	43 ± 2
α(-1064 nm; 1064 nm)	44 ± 1	42 ± 3	44 ± 1	44 ± 1
α(-910 nm; 910 nm)	42 ± 3	44 ± 2	43 ± 2	42 ± 3
α(-830 nm; 830 nm)	44 ± 2	43 ± 2	42 ± 3	43 ± 2
λ_h	340 ± 20	340 ± 20	340 ± 10	*340 ± 10*
λ_e	440 ± 40	430 ± 50	440 ± 30	440 ± 30
V_{exc} (3.5 Å)	790 ± 40	810 ± 50	800 ± 30	790 ± 40
V_{exc} (4.0 Å)	800 ± 50	810 ± 40	790 ± 40	780 ± 30
V_{exc} (4.5 Å)	820 ± 30	780 ± 60	800 ± 40	770 ± 40

Table S27. Slopes (with errors) for 4S-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	30 ± 10	32 ± 8	*30 ± 10*	*32 ± 7*
$E_{SPE}(+)$	30 ± 10	32 ± 8	*30 ± 10*	*32 ± 7*
$E_{SPE}(-)$	30 ± 10	32 ± 8	*30 ± 10*	*32 ± 7*
I_p	0.1 ± 0.1	0.1 ± 0.2	0.10 ± 0.09	0.1 ± 0.1
E_a	**0.11 ± 0.01**	**0.2 ± 0.01**	0.09 ± 0.02	**0.14 ± 0.01**
E_{HOMO}	-0.06 ± 0.03	-0.09 ± 0.06	-0.06 ± 0.02	-0.08 ± 0.04
E_{LUMO}	0.06 ± 0.02	0.09 ± 0.03	0.05 ± 0.02	0.07 ± 0.03
E_g	0.12 ± 0.03	0.18 ± 0.05	*0.10 ± 0.02*	*0.15 ± 0.03*
ΔH_f	800 ± 200	1200 ± 400	*700 ± 100*	*1000 ± 200*
ΔG_f	800 ± 200	1100 ± 400	*700 ± 100*	*1000 ± 200*
E_{Abs}	0.16 ± 0.02	0.24 ± 0.03	0.13 ± 0.02	0.20 ± 0.03
E_{Em}	0.13 ± 0.04	0.18 ± 0.08	0.11 ± 0.03	0.16 ± 0.04
α(0;0)	-2.4 ± 0.6	-4 ± 1	-2.1 ± 0.4	-3.0 ± 0.5
α(-1907 nm; 1907 nm)	-2.3 ± 0.4	-4 ± 1	-2.0 ± 0.6	-3.2 ± 0.3
α(-1370 nm; 1370 nm)	-2.5 ± 0.7	-4 ± 1	-2.0 ± 0.5	-3.1 ± 0.3
α(-1064 nm; 1064 nm)	-2.3 ± 0.5	-4 ± 1	-2.3 ± 0.6	-3.3 ± 0.4
α(-910 nm; 910 nm)	-2.2 ± 0.5	-4 ± 1	-2.2 ± 0.4	-3.0 ± 0.5
α(-830 nm; 830 nm)	-2.5 ± 0.7	-4 ± 1	-2.1 ± 0.5	-3.1 ± 0.5
λ_h	-20 ± 5	-30 ± 10	-18 ± 3	*-24 ± 5*
λ_e	-40 ± 10	-60 ± 20	-39 ± 7	-50 ± 10
V_{exc} (3.5 Å)	70 ± 10	110 ± 30	62 ± 9	90 ± 10
V_{exc} (4.0 Å)	70 ± 20	110 ± 40	62 ± 8	91 ± 7
V_{exc} (4.5 Å)	70 ± 10	110 ± 40	62 ± 9	91 ± 8

Table S28. Intercepts (with errors) for 5O-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	-1100 ± 40	-1100 ± 40	*-1100 ± 40*	*-1100 ± 40*
$E_{SPE}(+)$	-1100 ± 40	-1100 ± 40	*-1100 ± 40*	*-1100 ± 40*
$E_{SPE}(-)$	-1100 ± 40	-1100 ± 40	*-1100 ± 40*	*-1100 ± 40*
I_p	6.4 ± 0.1	6.4 ± 0.1	*6.4 ± 0.1*	6.40 ± 0.0
E_a	*-1.01 ± 0.04*	-1.01 ± 0.04	-0.99 ± 0.05	-0.99 ± 0.05
E_{HOMO}	-5.3 ± 0.1	-5.4 ± 0.1	-5.33 ±0.09	-5.32 ± 0.08
E_{LUMO}	-2.03 ± 0.06	-2.03 ± 0.05	-2.02 ± 0.06	-2.03 ± 0.06
E_g	**3.27 ± 0.04**	**3.28 ± 0.06**	**3.30 ± 0.04**	**3.29 ± 0.03**
ΔH_f	-20700 ± 900	-20600 ± 900	*-20400 ± 900*	*-20600 ± 900*
ΔG_f	-19300 ± 800	-19200 ± 800	*-19100 ± 900*	*-19200 ± 800*
E_{Abs}	3.26 ± 0.06	3.26 ± 0.07	3.29 ± 0.08	3.27 ± 0.07
E_{Em}	2.98 ± 0.06	3.00 ± 0.07	3.02 ± 0.0	3.00 ± 0.07
α(0;0)	53 ± 2	53 ±2	52 ± 2	52 ± 2
α(-1907 nm; 1907 nm)	54 ± 3	52 ±1	54 ± 1	53 ± 1
α(-1370 nm; 1370 nm)	52 ± 1	54 ±3	52 ± 3	52 ± 2
α(-1064 nm; 1064 nm)	52 ± 2	53 ±2	52 ± 3	54 ± 3
α(-910 nm; 910 nm)	53 ± 3	52 ±4	51 ± 1	53 ± 1
α(-830 nm; 830 nm)	54 ± 2	54 ±1	53 ± 2	52 ± 3
λ_h	240 ± 20	240 ± 20	240 ± 20	240 ± 20
λ_e	250 ± 20	250 ± 20	240 ± 20	250 ± 20
V_{exc} (3.5 Å)	840 ± 30	840 ± 40	**697 ± 4**	**850 ± 10**
V_{exc} (4.0 Å)	850 ± 30	830 ± 30	**689 ± 6**	**848 ± 8**
V_{exc} (4.5 Å)	840 ± 40	840 ± 30	**695 ± 3**	**849 ± 9**

Table S29. Slopes (with errors) for 5O-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	27 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
$E_{SPE}(+)$	27 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
$E_{SPE}(-)$	27 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
I_p	0.01 ± 0.02	0.16 ± 0.04	*0.06± 0.01*	0.11 ± 0.02
E_a	*0.041 ± 0.008*	0.07 ± 0.01	0.026 ± 0.006	0.04 ± 0.01
E_{HOMO}	-0.08 ± 0.02	-0.12 ± 0.04	*-0.05 ± 0.01*	*-0.08 ± 0.02*
E_{LUMO}	0.02 ± 0.01	0.03 ± 0.01	0.011 ± 0.07	0.02 ± 0.01
E_g	**0.094 ± 0.008**	**0.16 ± 0.02**	**0.061 ± 0.005**	**0.104 ± 0.007**
ΔH_f	600 ± 200	1000 ± 300	*406 ± 100*	*700 ± 200*
ΔG_f	600 ± 200	1000 ± 300	*400 ± 100*	*600 ± 200*
E_{Abs}	0.09 ± 0.01	0.15 ± 0.02	0.06 ± 0.01	0.10 ± 0.01
E_{Em}	0.09 ± 0.01	0.14 ± 0.02	0.05 ± 0.01	0.09 ± 0.01
α(0;0)	-2.0 ± 0.4	-3.3 ± 0.7	-1.3 ± 0.3	-2.2 ± 0.5
α(-1907 nm; 1907 nm)	-1.9 ± 0.5	-3.2 ± 0.8	-1.4 ± 0.4	-2.1 ± 0.4
α(-1370 nm; 1370 nm)	-2.0 ± 0.3	-3.3 ± 0.6	-1.4 ± 0.4	-2.3 ± 0.4
α(-1064 nm; 1064 nm)	-2.1 ± 0.4	-3.4 ± 0.5	-1.2 ± 0.2	-2.2 ± 0.3
α(-910 nm; 910 nm)	-2.0 ± 0.3	-3.3 ± 0.6	-1.3 ± 0.4	-2.3 ± 0.5
α(-830 nm; 830 nm)	-1.9 ± 0.3	-3.2 ± 0.7	-1.2 ± 0.3	-2.2 ± 0.4
λ_h	1 ± 3	2 ± 5	1 ± 2	1 ± 3
λ_e	-5 ± 3	-8 ± 6	-3 ± 2	5 ± 4
V_{exc} (3.5 Å)	490 ± 5	800 ± 10	**330 ± 1**	**550 ± 2**
V_{exc} (4.0 Å)	493 ± 4	820 ± 10	**333 ± 2**	**548 ± 3**
V_{exc} (4.5 Å)	492 ± 6	810 ± 10	**329 ± 1**	**551 ± 2**

Table S30. Intercepts (with errors) for 5S-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	-1700 ± 40	-1700 ± 40	*-1700 ± 40*	*-1700 ± 40*
$E_{SPE}(+)$	-1700 ± 40	-1700 ± 40	*-1700 ± 40*	*-1700 ± 40*
$E_{SPE}(-)$	-1700 ± 40	-1700 ± 40	*-1700 ± 40*	*-1700 ± 40*
I_p	6.5 ± 0.1	6.5 ± 0.1	6.54 ± 0.09	6.52 ± 0.09
E_a	**-1.18 ± 0.02**	**-1.18 ± 0.01**	-1.16 ± 0.04	-1.17 ± 0.04
E_{HOMO}	-5.5 ± 0.1	-5.6 ± 0.1	*-5.55 ± 0.09*	*-5.54 ± 0.09*
E_{LUMO}	-2.05 ± 0.03	-2.04 ± 0.02	-2.06 ± 0.04	-2.05 ± 0.03
E_g	3.49 ± 0.08	3.50 ± 0.09	3.51 ± 0.08	3.50 ± 0.07
ΔH_f	-21200 ± 900	-21100 ± 900	*-20900 ± 900*	*-21100 ± 900*
ΔG_f	-19800 ± 800	3.36 ± 0.09	*-19500 ± 900*	*-19600 ± 800*
E_{Abs}	3.35 ± 0.08	3.00 ± 0.07	3.37 ± 0.07	3.36 ± 0.06
E_{Em}	2.9 ± 0.1	2.93 ± 0.1	0.11534	2.9 ± 0.1
α(0;0)	57 ± 2	57 ± 2	56 ± 2	56 ± 2
α(-1907 nm; 1907 nm)	57 ± 1	55 ± 3	55 ± 1	57 ± 3
α(-1370 nm; 1370 nm)	56 ± 2	56 ± 3	57 ± 2	57 ± 2
α(-1064 nm; 1064 nm)	56 ± 3	58 ± 2	56 ± 3	55 ± 1
α(-910 nm; 910 nm)	58 ± 2	58 ± 4	54 ± 2	56 ± 2
α(-830 nm; 830 nm)	57 ± 2	55 ± 2	55 ± 2	55 ± 3
λ_h	**348 ± 6**	**347.9 ± 0.8**	**340 ± 14**	**340 ± 14**
λ_e	**421 ± 4**	**421 ± 6**	**415 ± 6**	**418 ± 7**
V_{exc} (3.5 Å)	770 ± 30	780 ± 40	670 ± 30	**782 ± 7**
V_{exc} (4.0 Å)	760 ± 30	770 ± 40	660 ± 20	**785 ± 8**
V_{exc} (4.5 Å)	770 ± 40	780 ± 50	650 ± 30	**783 ± 4**

Table S31. Slopes (with errors) for 5S-compounds' properties.

	F_{00}	F_{01}	F_{10}	F_{11}
$E_{SPE}(0)$	30 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
$E_{SPE}(+)$	30 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
$E_{SPE}(-)$	30 ± 7	40 ± 10	*17 ± 5*	*30 ± 8*
I_p	0.06 ± 0.02	0.11 ± 0.03	0.04 ± 0.01	0.08 ± 0.02
E_a	**0.057 ± 0.004**	**0.094 ± 0.003**	0.036 ± 0.005	0.062 ± 0.008
E_{HOMO}	-0.03 ± 0.02	-0.05 ± 0.03	-0.02 ± 0.01	-0.03 ± 0.02
E_{LUMO}	0.02 ± 0.01	0.03 ± 0.02	0.03 ± 0.01	0.02 ± 0.01
E_g	0.05 ± 0.02	0.09 ± 0.03	0.03 ± 0.01	0.06 ± 0.02
ΔH_f	600 ± 200	1000 ± 300	*400 ± 100*	*700 ± 200*
ΔG_f	600 ± 200	400 ± 200	*400 ± 100*	*600 ± 200*
E_{Abs}	0.08 ± 0.01	0.13 ± 0.03	0.052 ± 0.008	0.09 ± 0.01
E_{Em}	0.05 ± 0.02	0.09 ± 0.04	0.04 ± 0.01	0.06 ± 0.02
α(0;0)	-1.9 ± 0.4	-3.1 ± 0.8	-1.2 ± 0.3	-2.1 ± 0.5
α(-1907 nm; 1907 nm)	-1.9 ± 0.5	-3.2 ± 0.9	-1.3 ± 0.3	-2.0 ± 0.4
α(-1370 nm; 1370 nm)	-1.8 ± 0.5	-3.1 ± 0.8	-1.2 ± 0.4	-2.1 ± 0.5
α(-1064 nm; 1064 nm)	-1.9 ± 0.4	-3.1 ± 0.7	-1.1 ± 0.5	-2.3 ± 0.6
α(-910 nm; 910 nm)	-2.0 ± 0.3	-3.0 ± 0.7	-1.1 ± 0.2	-2.2 ± 0.4
α(-830 nm; 830 nm)	-2.0 ± 0.3	-3.2 ± 0.8	-1.3 ± 0.3	-2.1 ± 0.4
λ_h	**-23 ± 1**	**-38.1 ± 0.3**	**-15 ± 2**	**-25 ±3**
λ_e	**-19.6 ± 0.7**	**-32 ± 2**	**-12.8 ± 0.8**	**-21 ± 1**
V_{exc} (3.5 Å)	52 ± 4	90 ± 10	30 ± 3	**59 ± 1**
V_{exc} (4.0 Å)	55 ± 5	90 ± 10	32 ± 2	**57 ± 1**
V_{exc} (4.5 Å)	54 ± 2	90 ± 10	29 ± 3	**58 ± 1**

Footnote to Tables S24 – S31

$E_{SPE}(0)$, $E_{SPE}(+)$, $E_{SPE}(-)$ - single-point energies at neutral, cationic and anionic states respectively; I_p - ionisation potential; E_a - electron affinity; E_{HOMO}, E_{LUMO} - energies of HOMO, LUMO respectively; E_g - electron gap between boundary orbitals; E_{abs}, E_{em} - transition energy for the brightest absorption electronic band and $S_1 \rightarrow S_0$ emission (fluorescence) energy; α(0;0), α(-1907 nm; 1907 nm), α(-1370 nm; 1370 nm), α(-1064 nm; 1064 nm), α(-910 nm; 910 nm), α(-830 nm; 830 nm) - first static and dynamic molecular electric isotropic polarisabilities; λ_h - hole reorganisation energy; λ_e - electron reorganisation energy; V_{exc} (3.5 Å), V_{exc} (4.0 Å), V_{exc} (4.5 Å) - exciton couplings evaluated different distances.

4. Graphical representation of correlations with F-index

Legend of graphical representation

Correlations of 4O (filled red squares), 4S (filled blue circles), 5O (red squares) and 5S (blue circles) compound groups with: (a) F_{00} index; (b) F_{01} index; (c) F_{10} index; (d) F_{11} index correlation. Regression lines shown with the respective colours in a solid line for 4-ringed compounds and in a hyphened line for 5-ringed compounds.

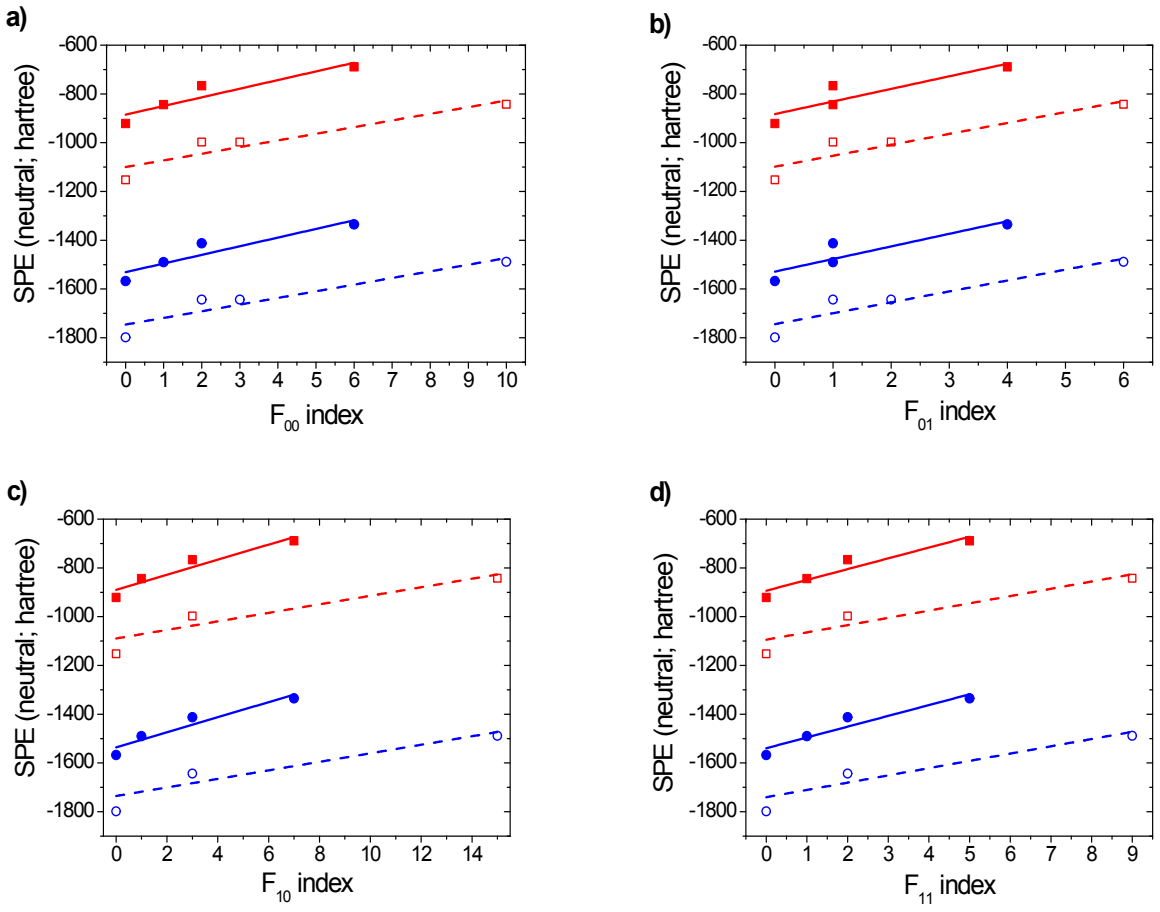

Figure S1. Single-point energy in neutral state.

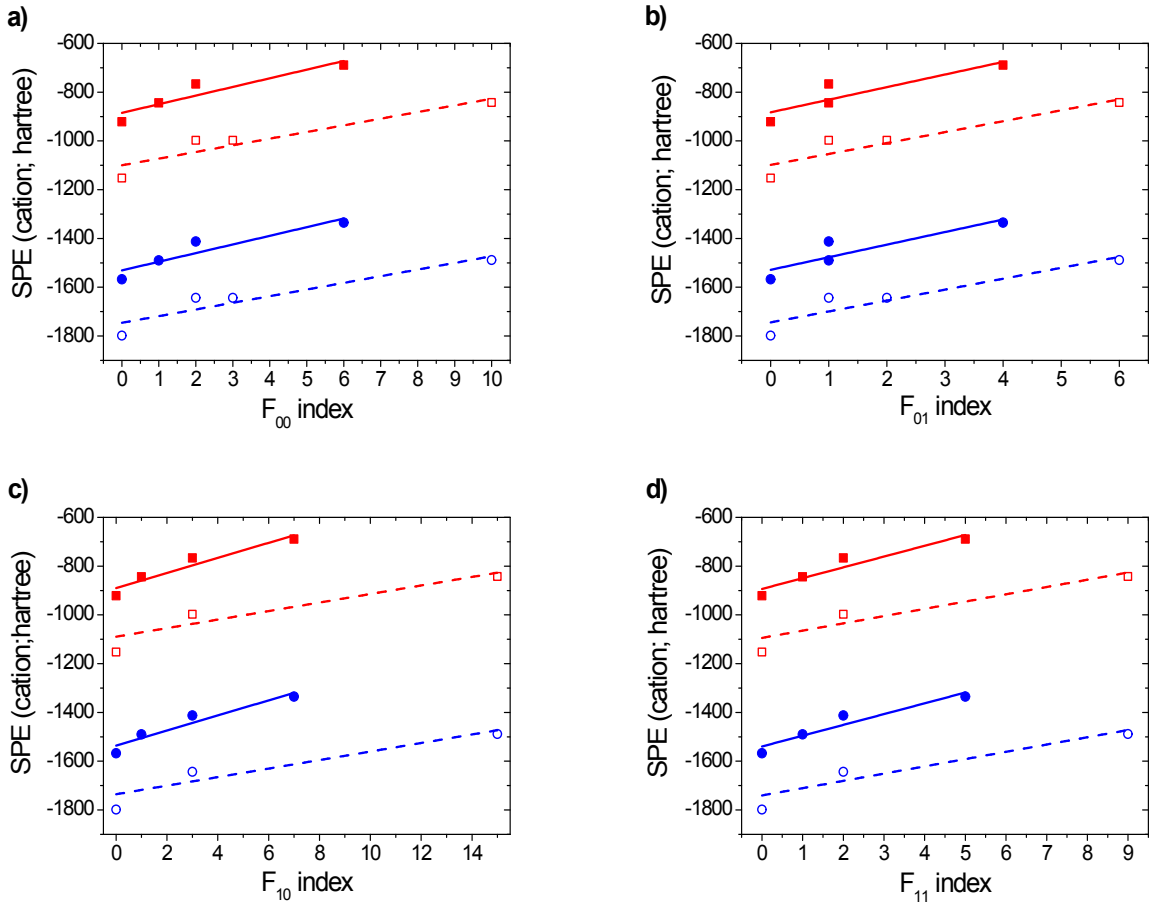

Figure S2. Single-point energy in cationic state.

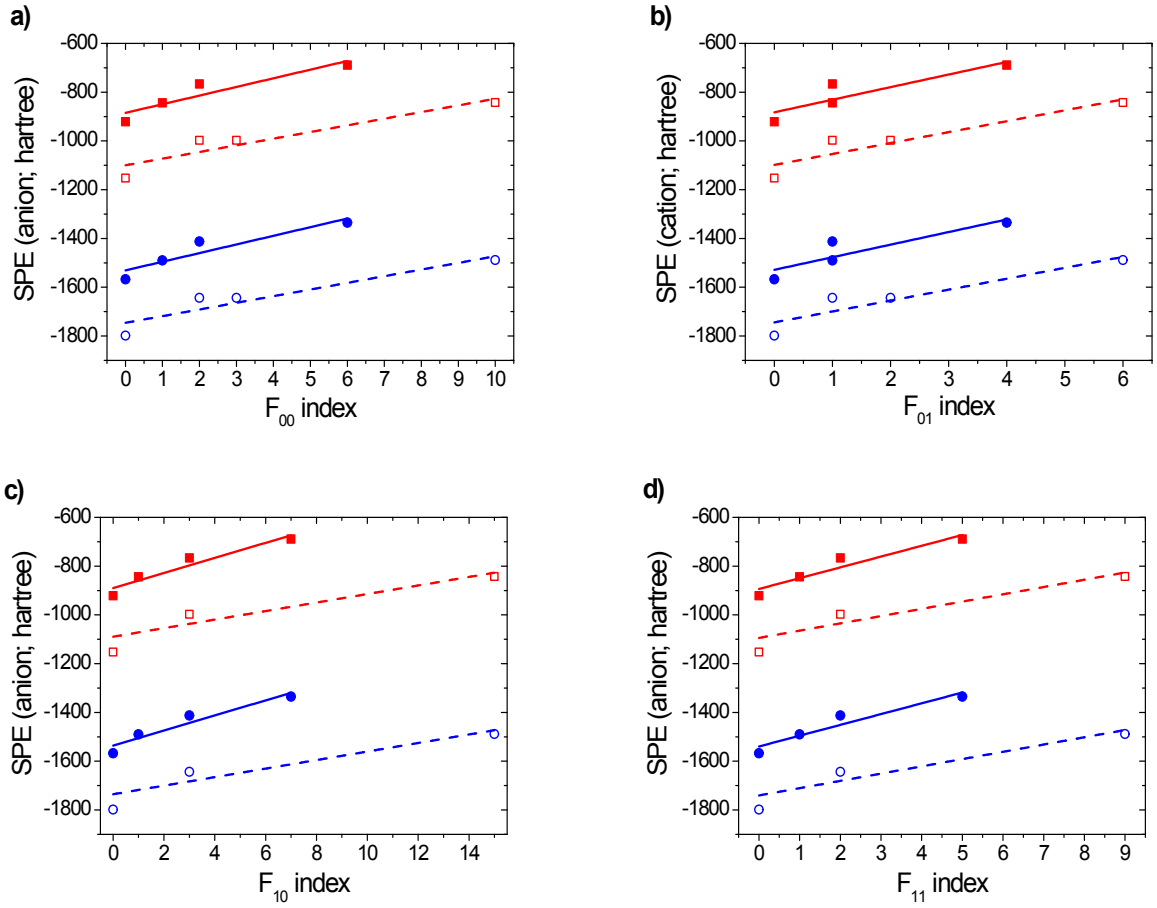

Figure S3. Single-point energy in anionic state.

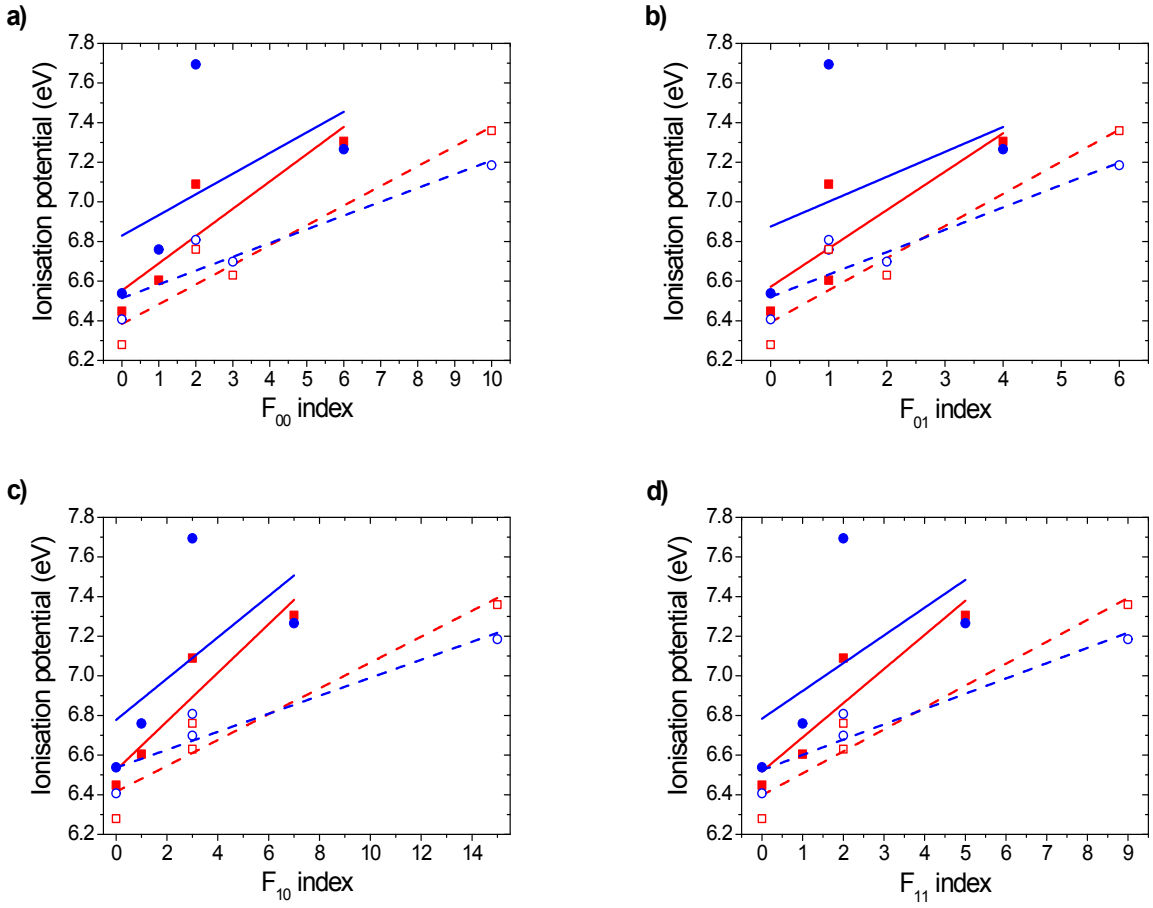

Figure S4. Ionisation potential.

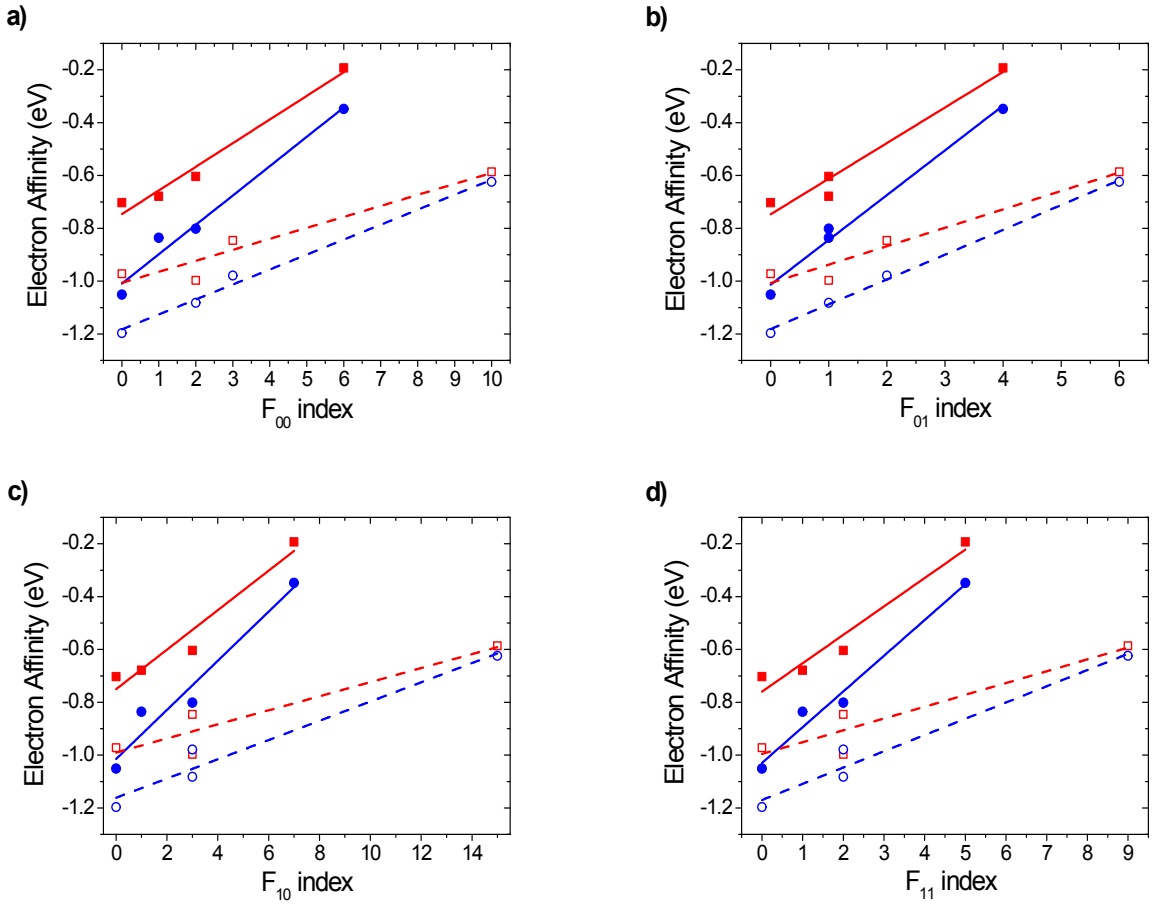

Figure S5. Electron affinity.

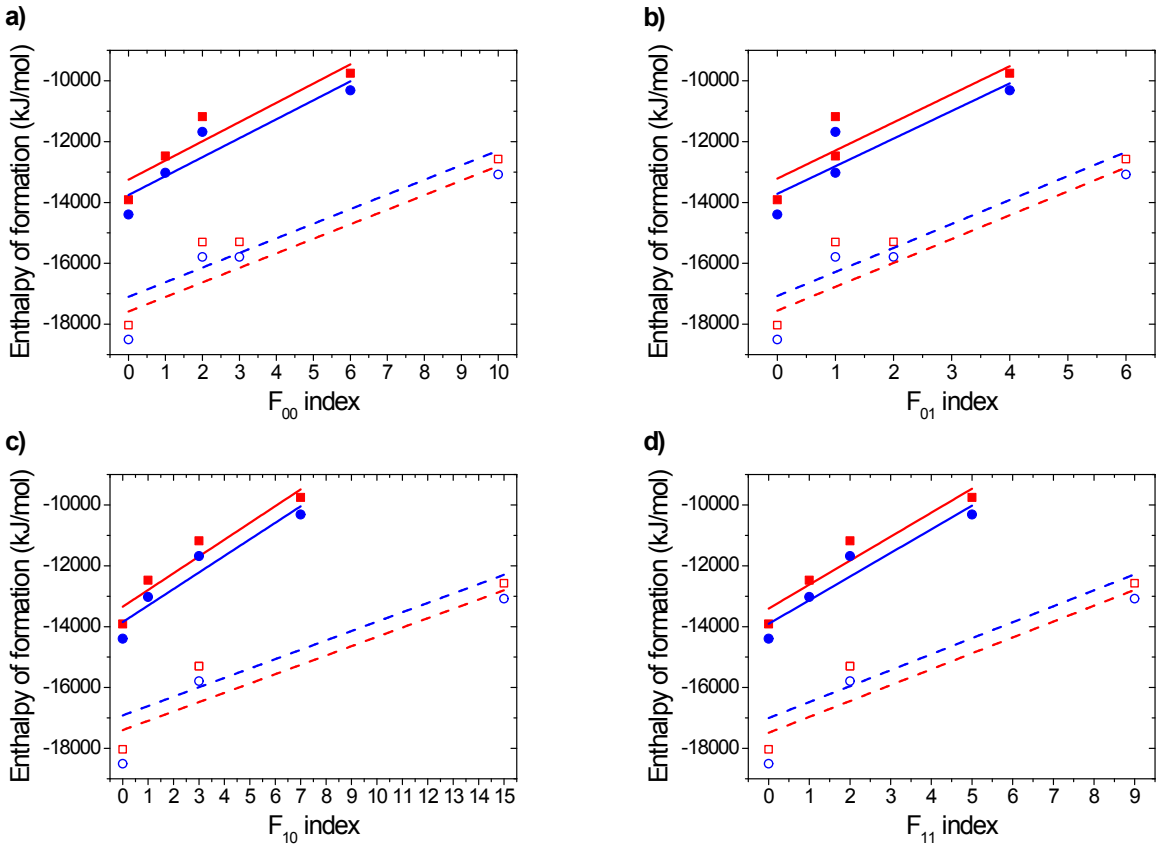

Figure S6. Enthalpy of formation.

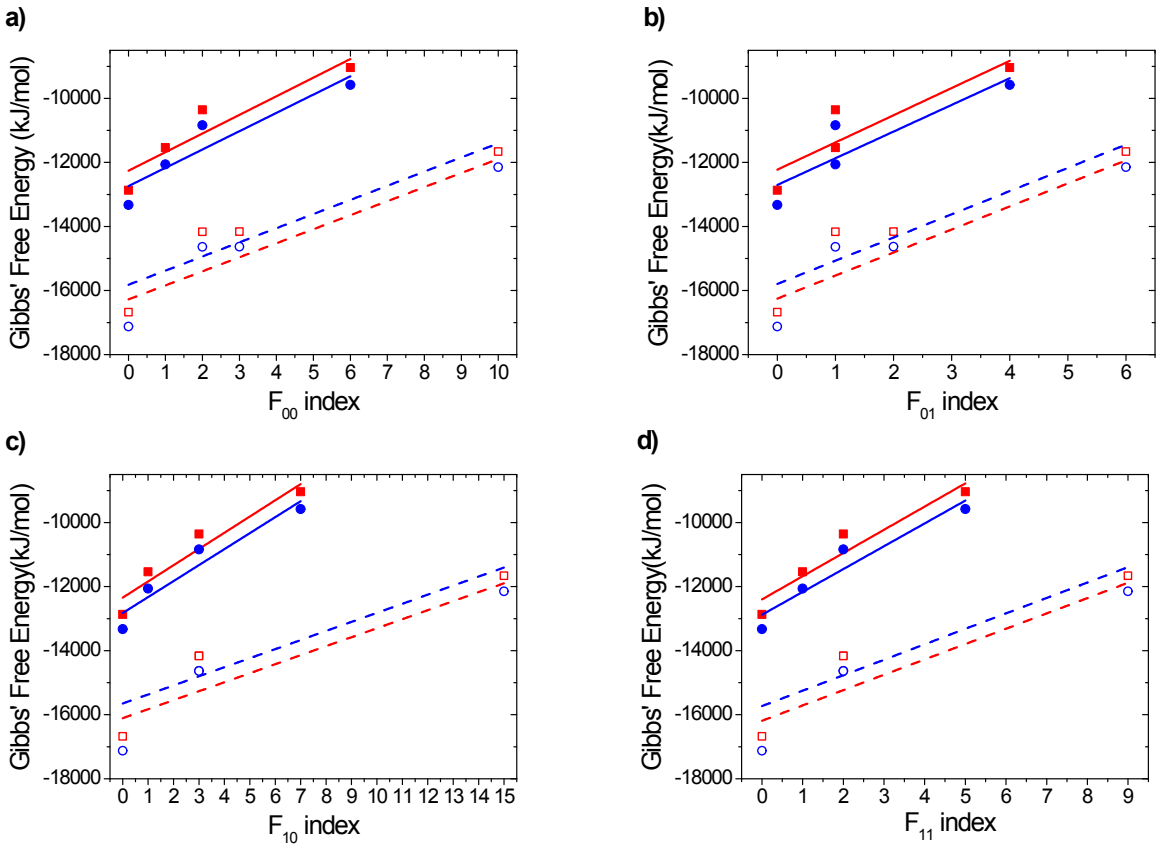

Figure S7. Gibbs' free energy of formation.

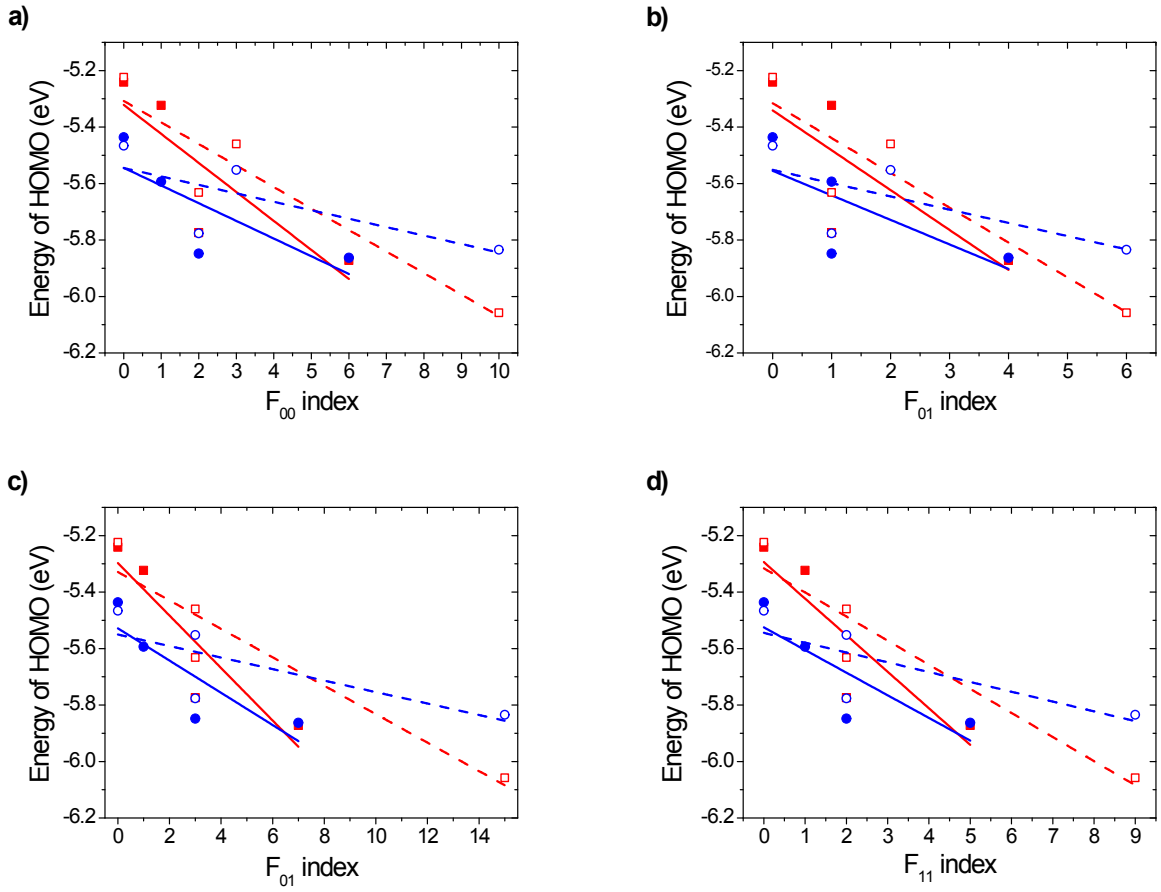

Figure S8. Energy of HOMO.

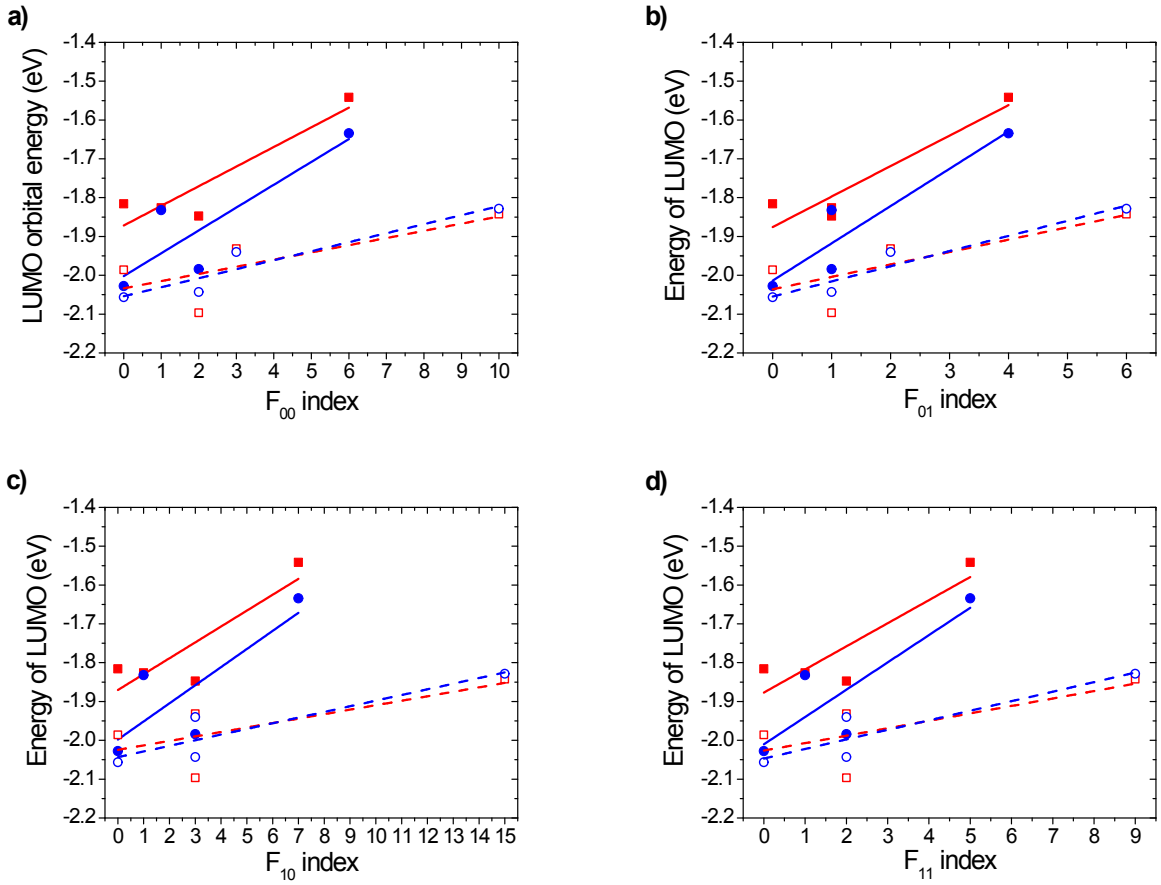

Figure S9. Energy of LUMO.

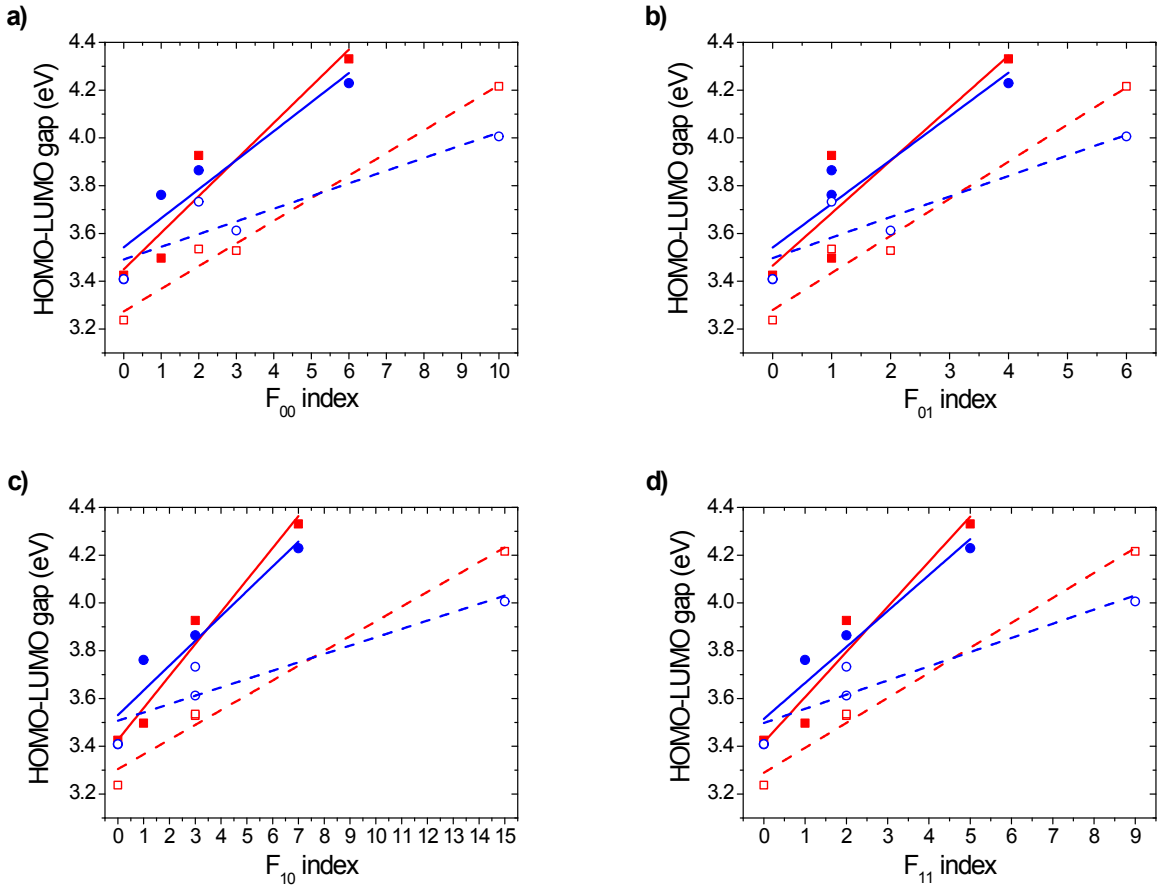

Figure S10. HOMO-LUMO gap.

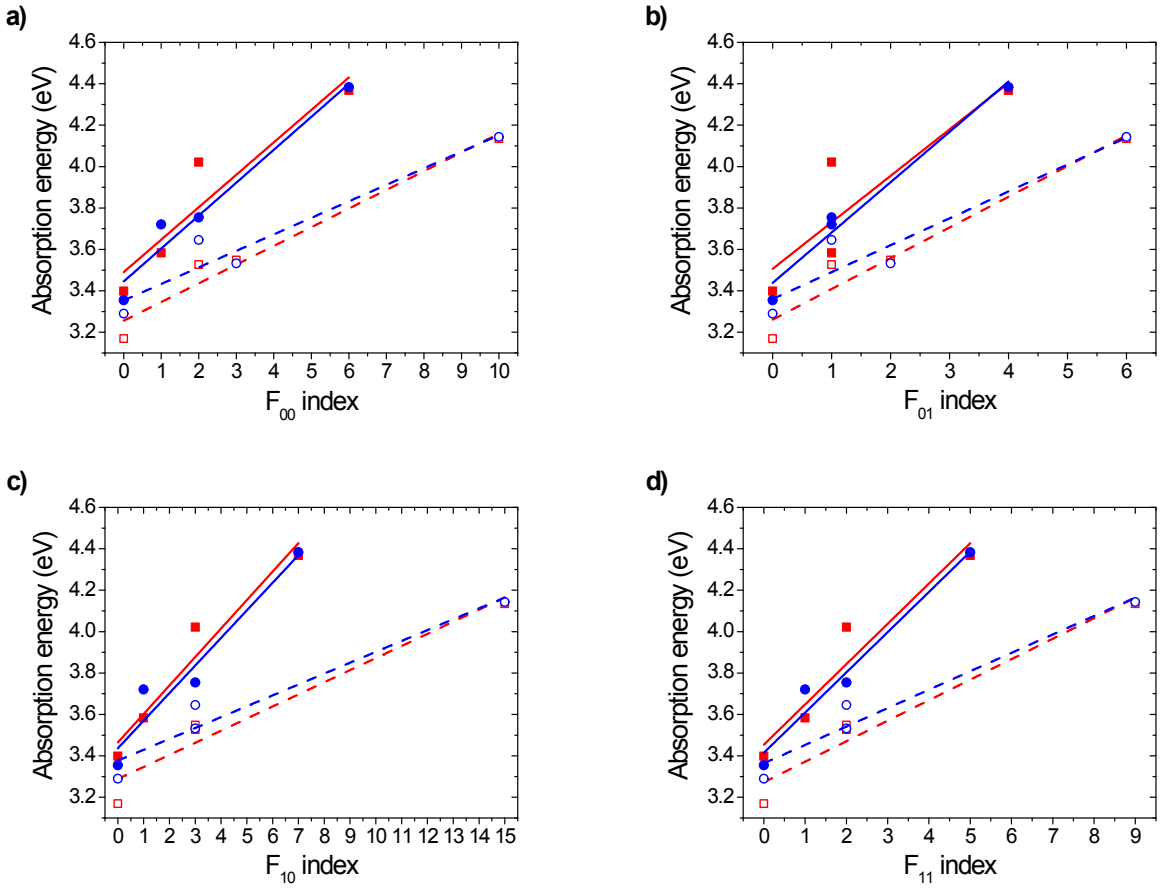

Figure S11. Absorption energy for the brightest $S_0 \rightarrow S_n$ transition.

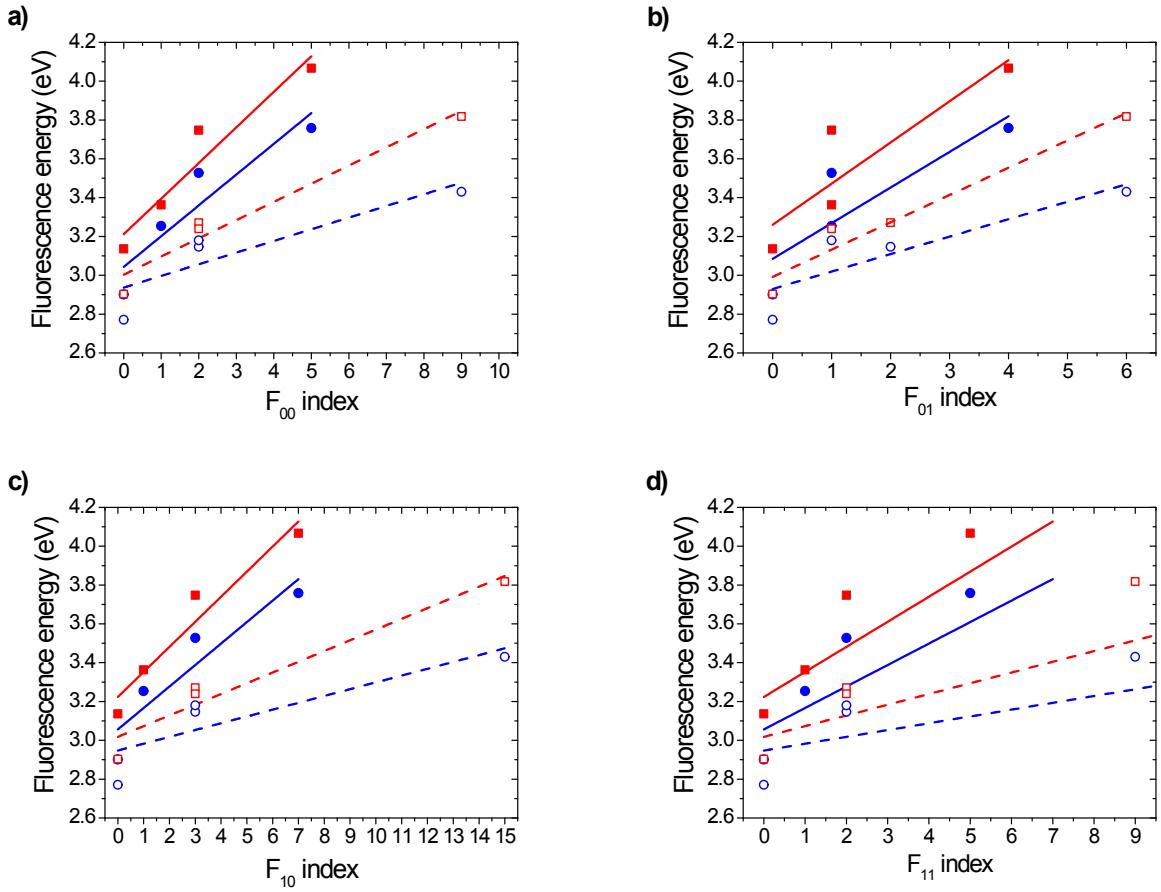

Figure S12. Fluorescence energy.

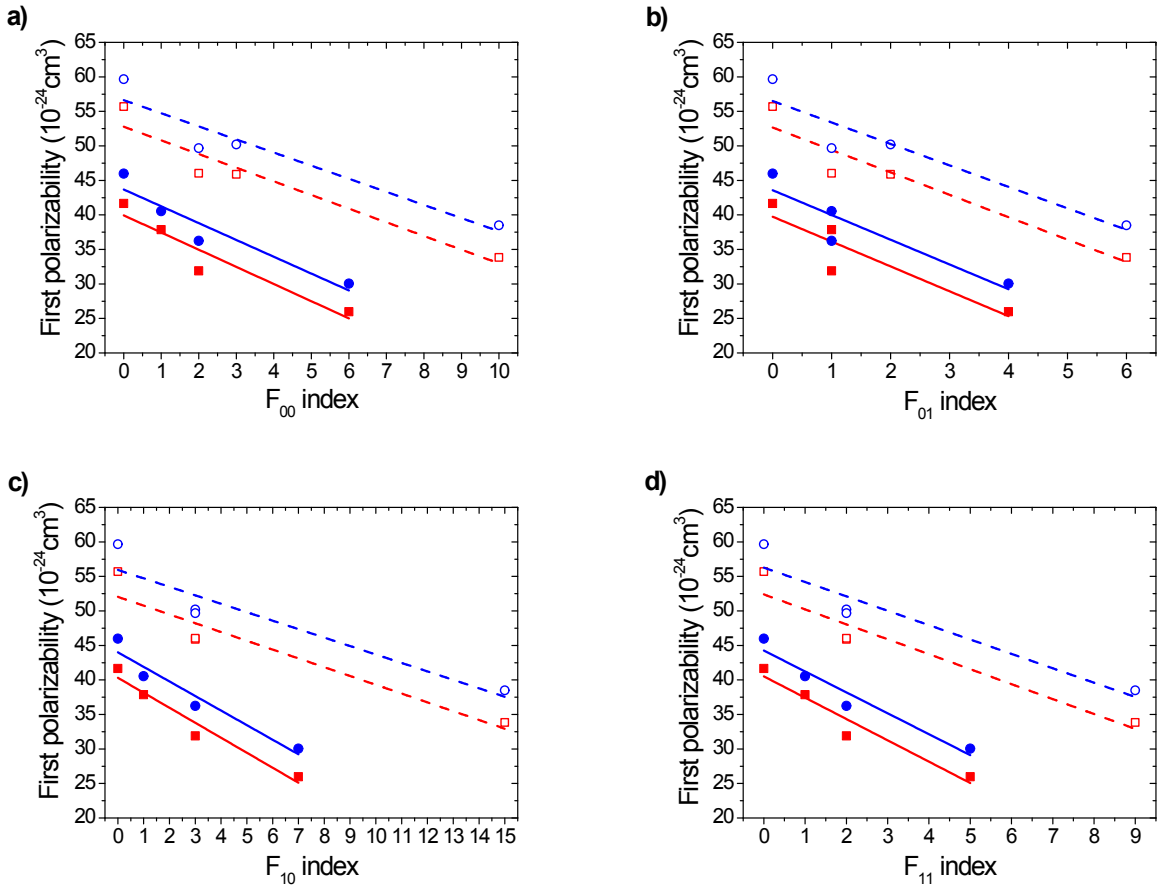

Figure S13. First static electric polarisability.

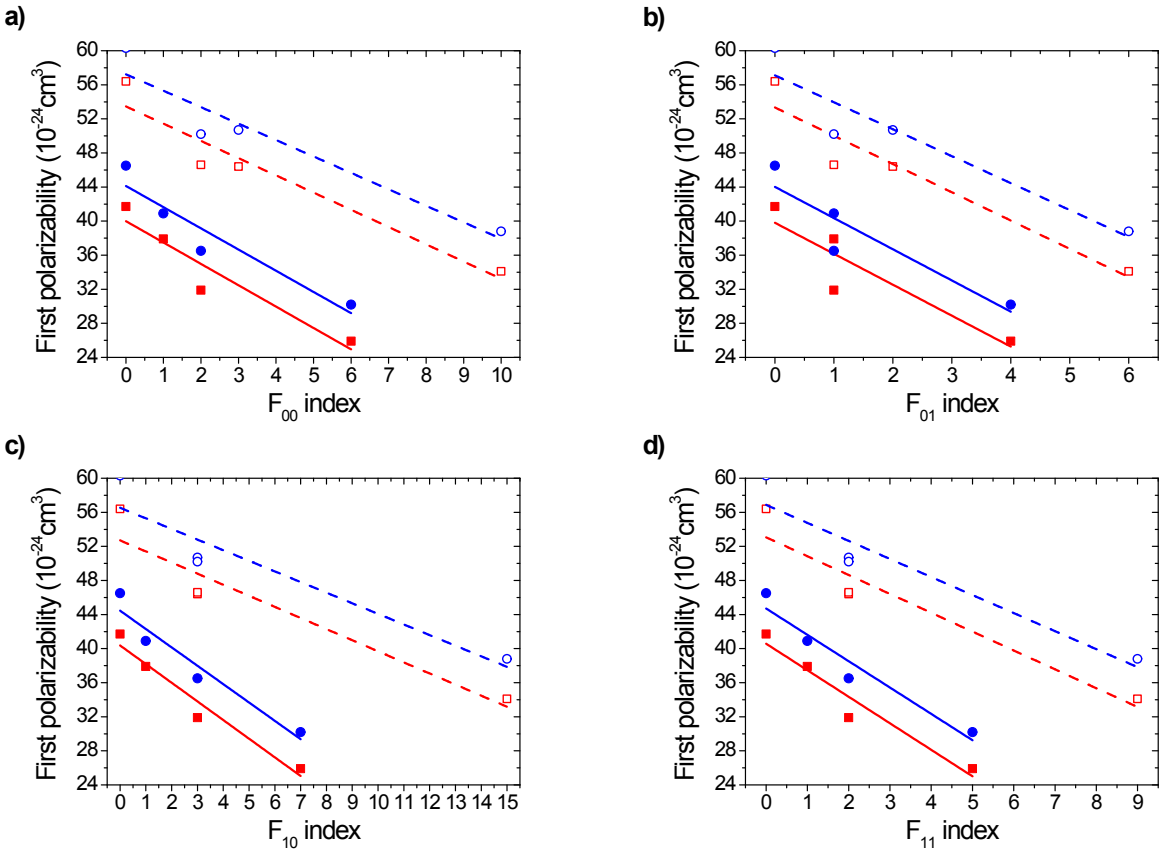

Figure S14. First dynamic electric polarisability (at λ = 1970 nm).

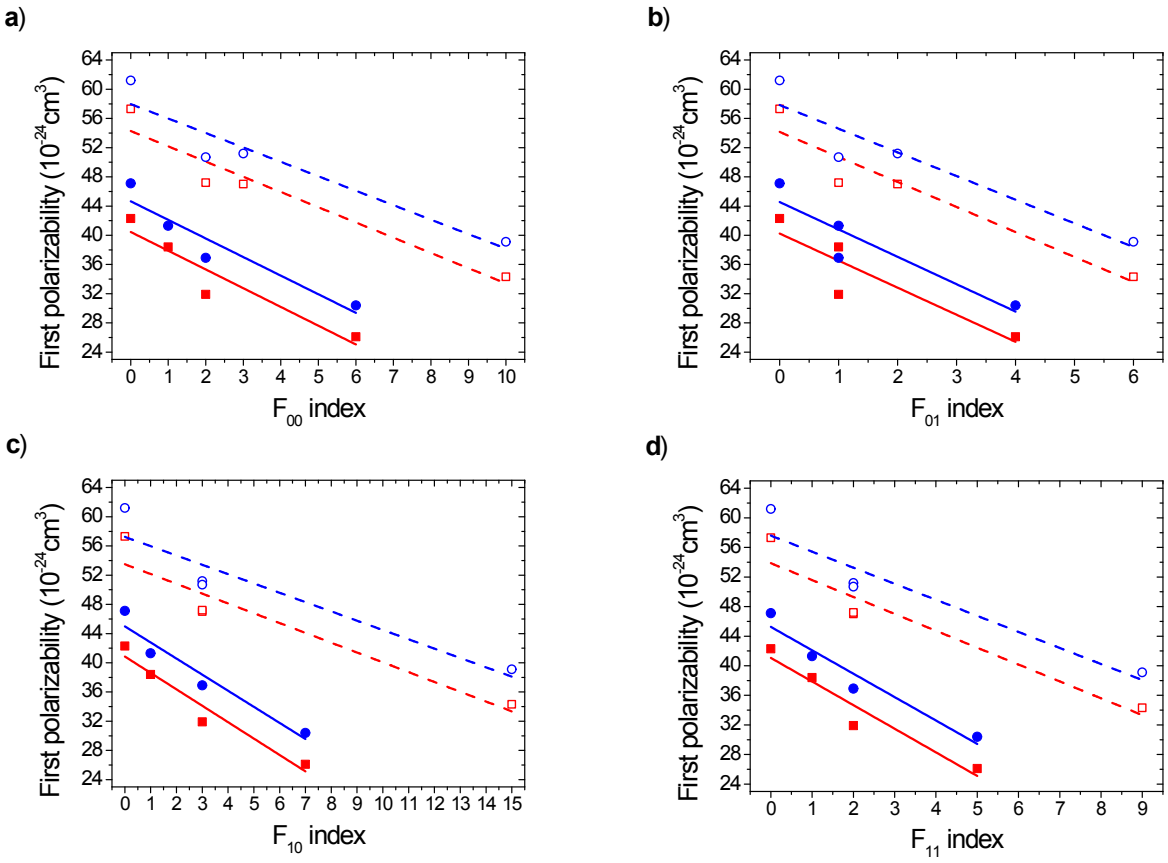

Figure S15. First dynamic electric polarisability (at λ = 1370 nm).

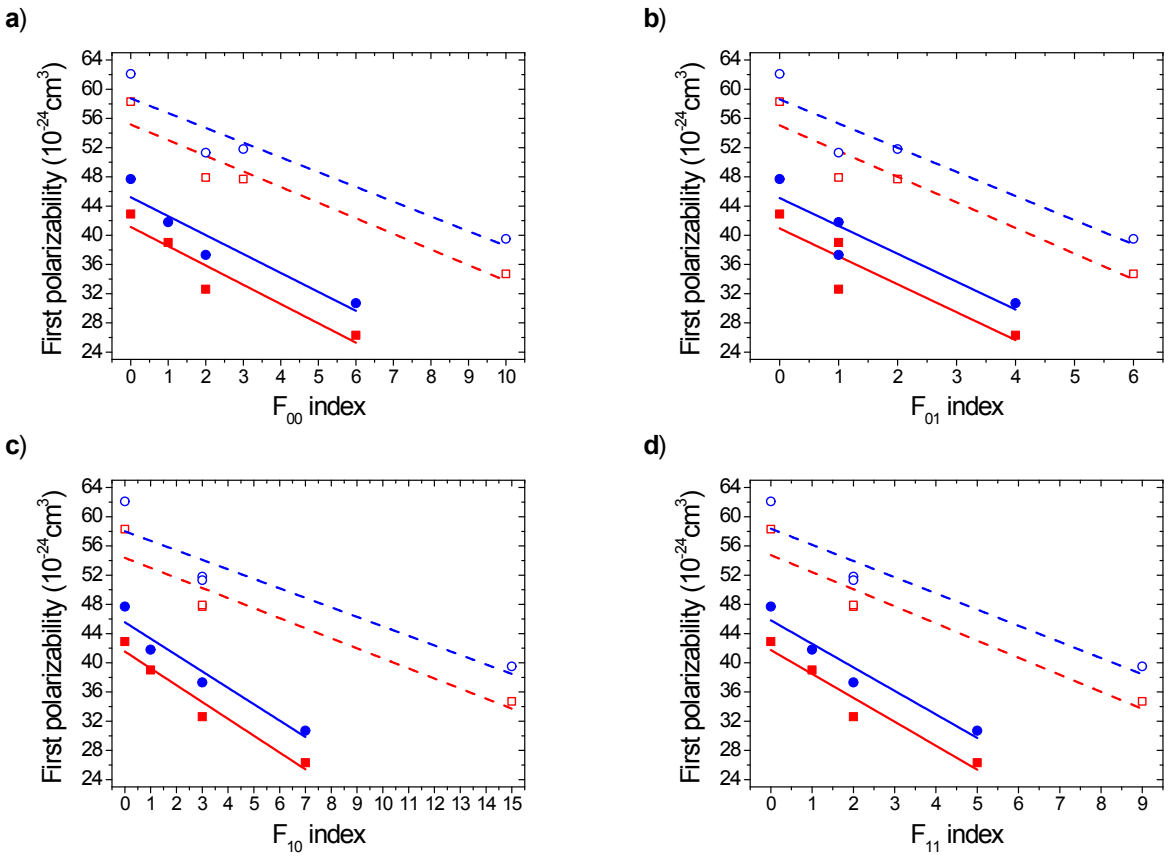

Figure S16. First dynamic electric polarisability (at λ = 1064 nm).

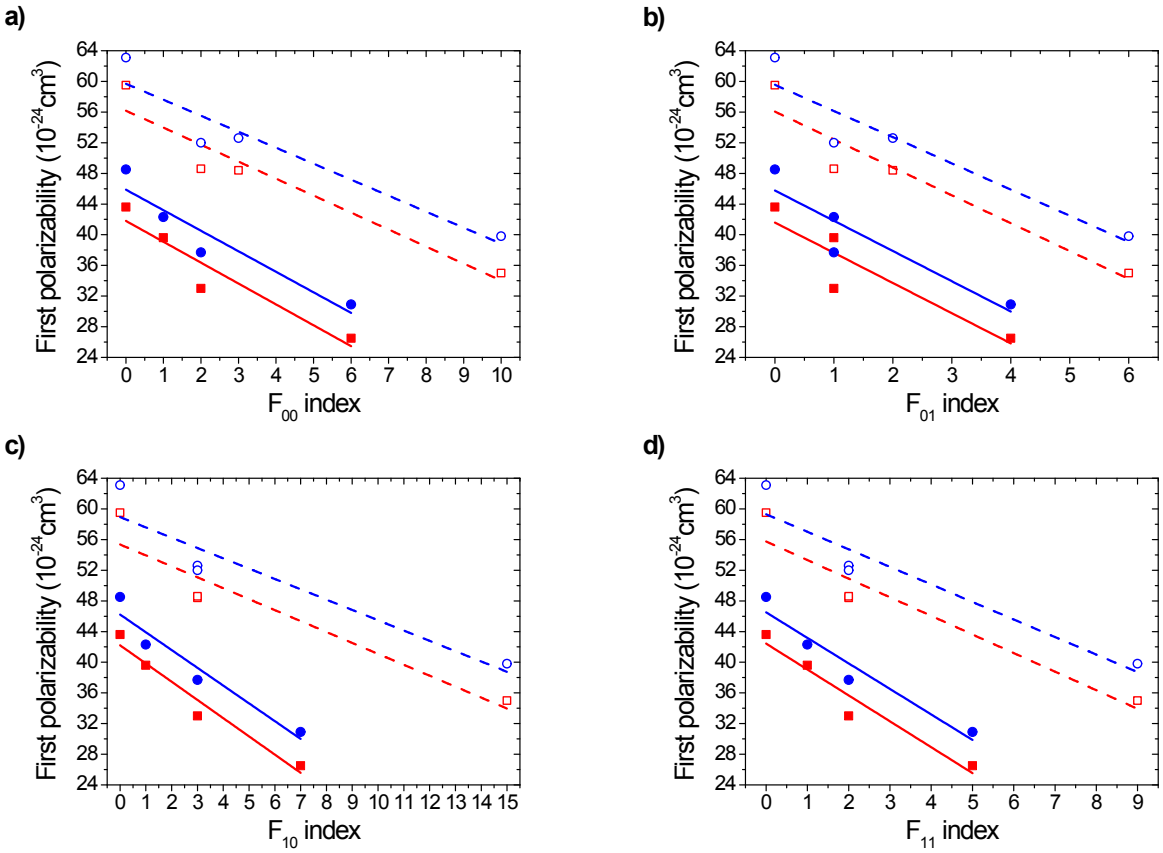

Figure S17. First dynamic electric polarisability (at λ = 910 nm).

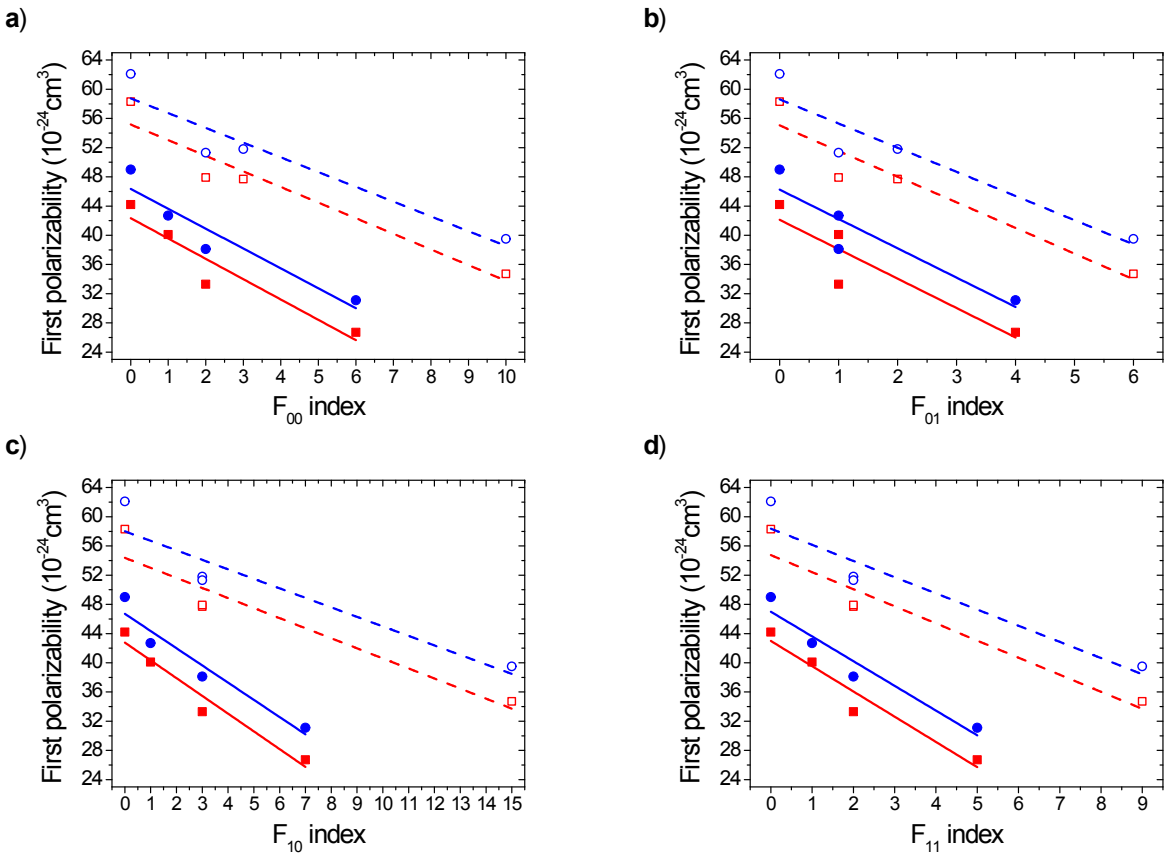

Figure S18. First dynamic electric polarisability (at λ = 830 nm).

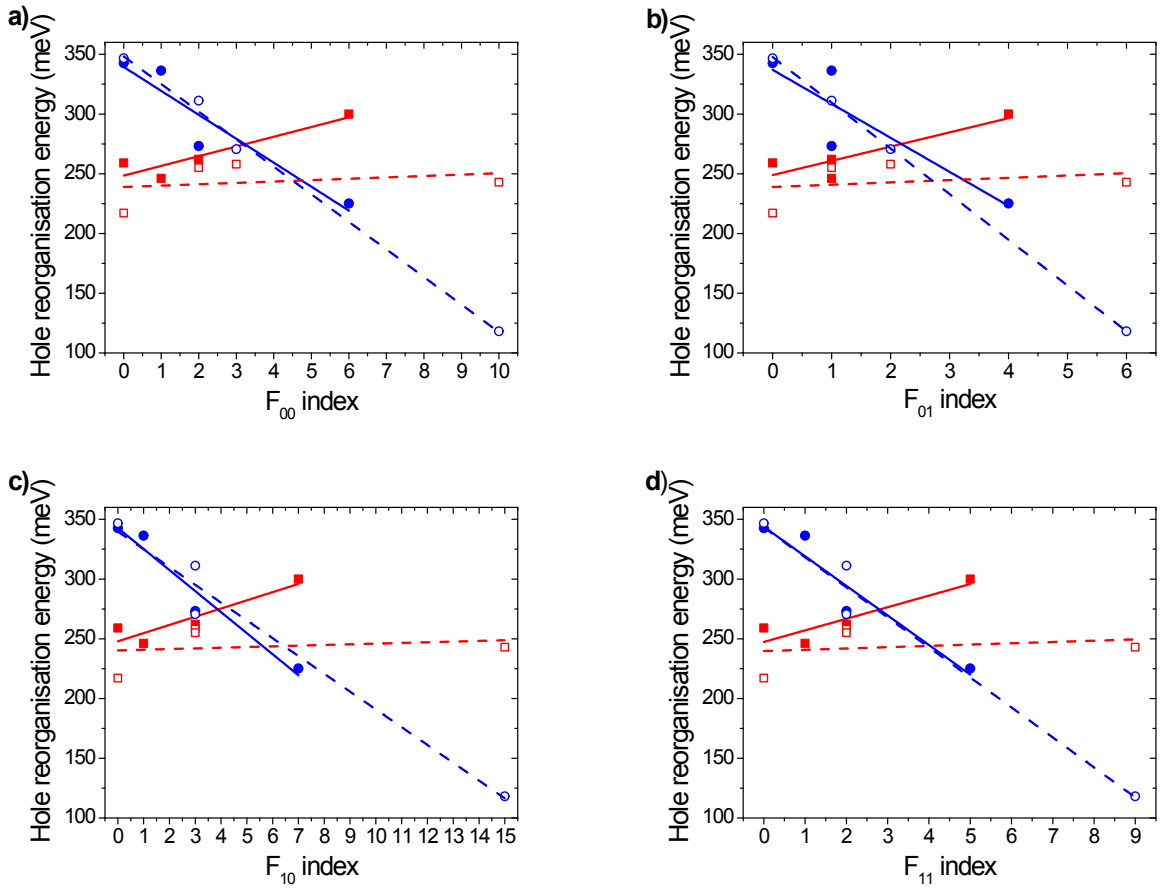

Figure S19. Hole reorganisation energy.

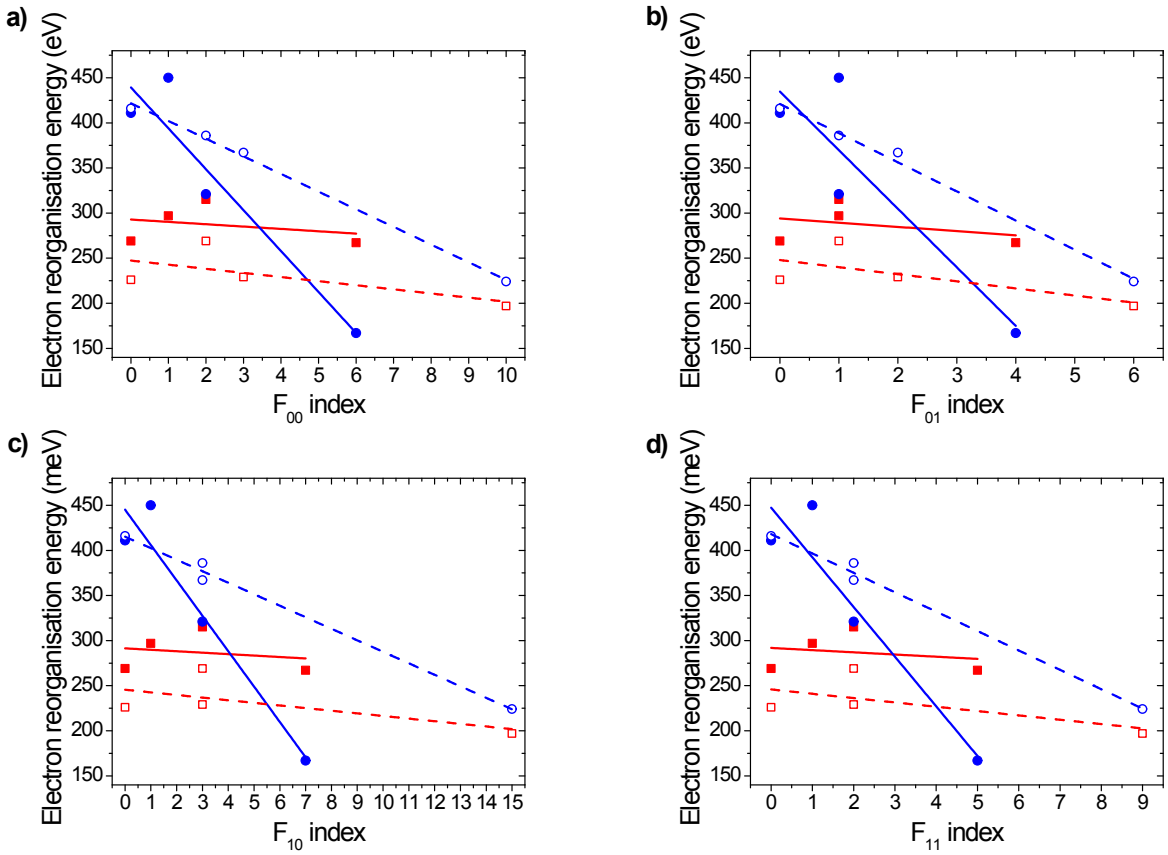

Figure S20. Electron reorganisation energy.

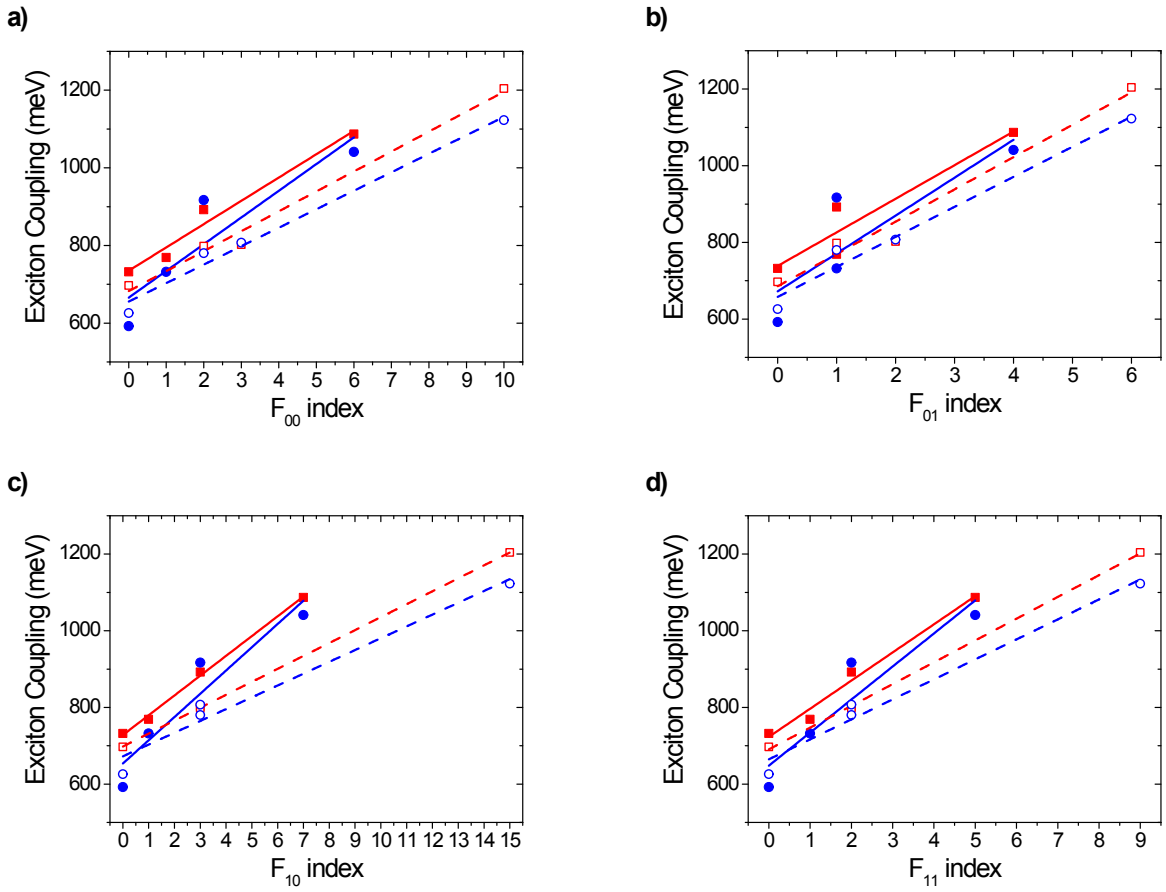

Figure S21. Exciton coupling (distance equal to 3.5 Å).

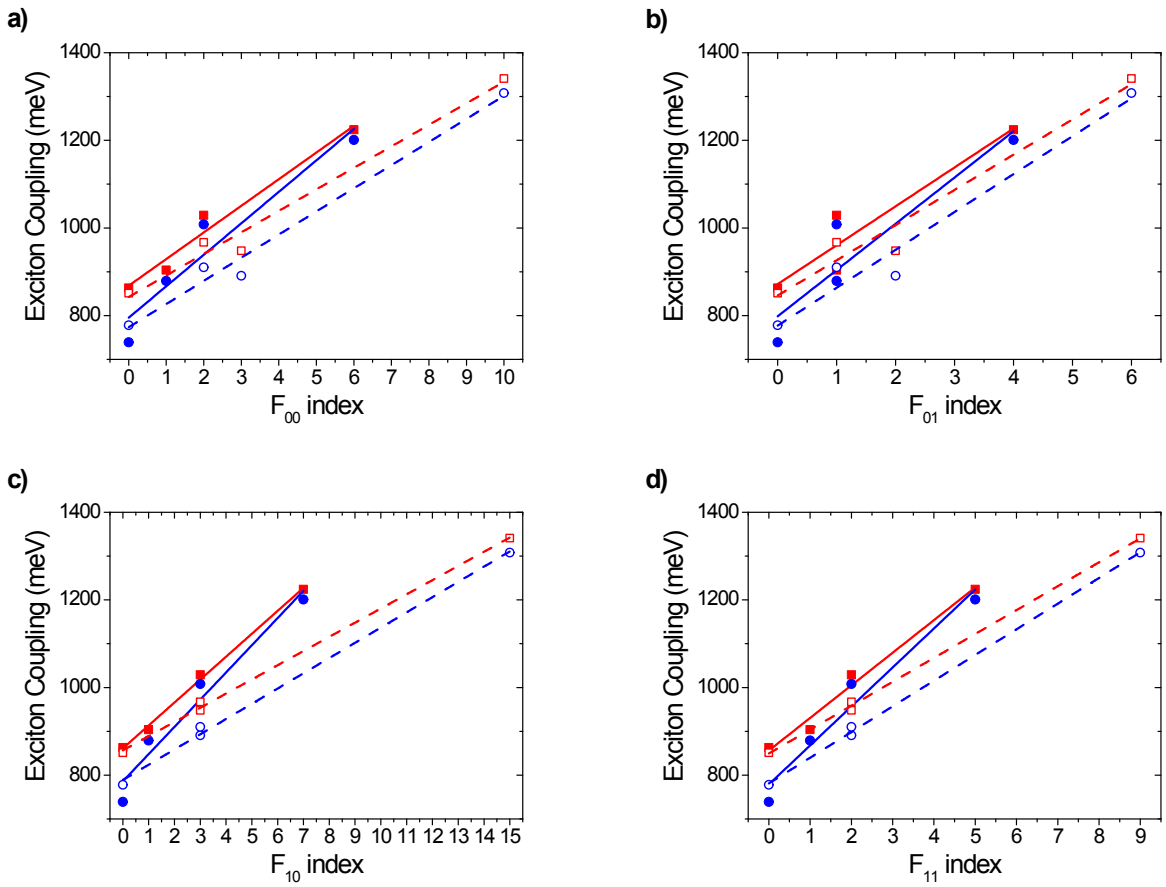

Figure S22. Exciton coupling (distance equal to 4.0 Å).

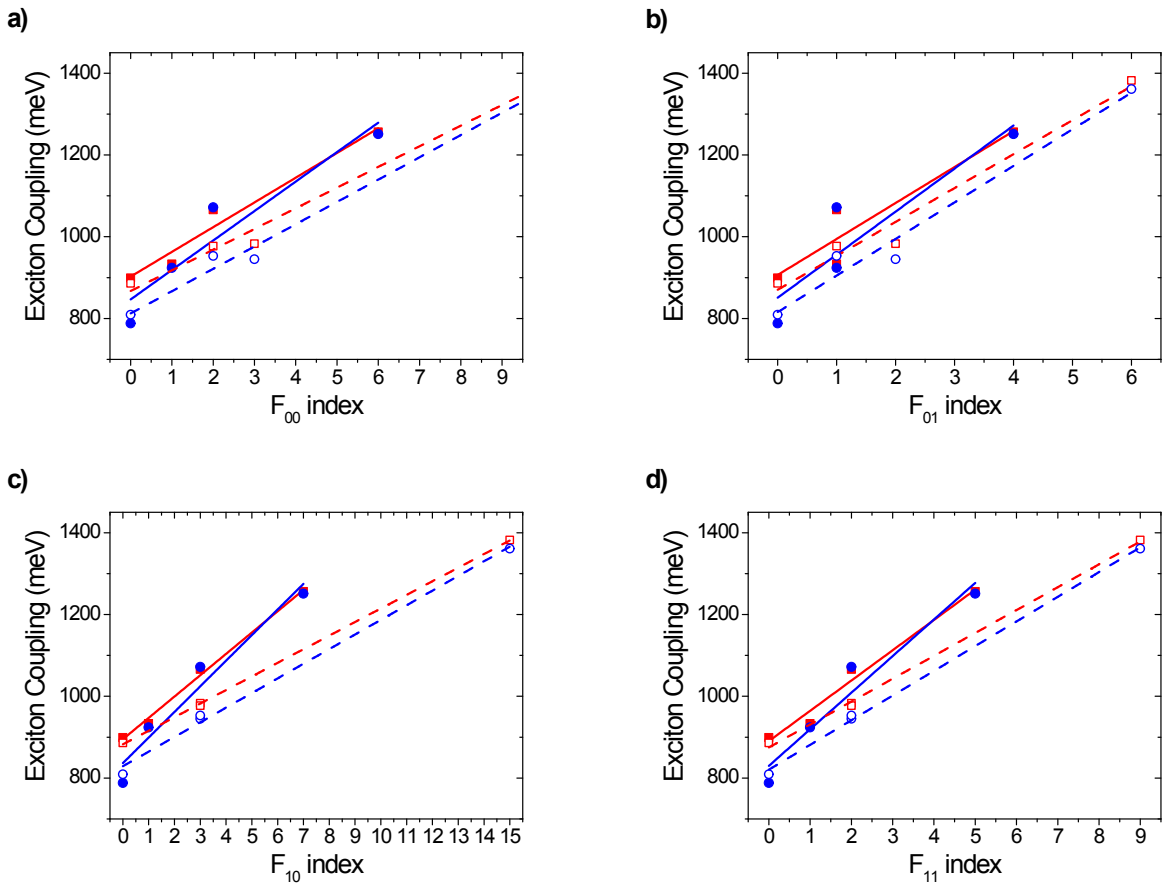

Figure S23. Exciton coupling (distance equal to 4.5 Å).

5. Atomic coordinates of optimised structures of investigated compounds

5.1 Neutral ground state

4Oa compound

C	2.79905500	-0.46414500	-0.78060200
C	1.53007600	-1.05373000	-0.52849600
C	0.68337600	-0.02423300	-0.20808000
C	2.66096800	0.88893800	-0.60159600
C	-0.70383700	0.03462800	0.14261900
C	-2.68142900	-0.87854400	0.53613500
C	-2.81951600	0.47454000	0.71514100
C	-1.55053700	1.06412400	0.46303600
C	-3.59595600	-2.00478700	0.64274500
C	3.57549500	2.01518200	-0.70820600
C	-3.16293200	-3.31707400	0.38993400
C	-4.04709500	-4.38610800	0.49510200
C	-5.37704200	-4.17156700	0.85310000
C	-5.81708300	-2.87140400	1.10638000
C	-4.93926500	-1.79965800	1.00316600
C	3.14247100	3.32746800	-0.45539500
C	4.02663400	4.39650300	-0.56056200
C	5.35658100	4.18196100	-0.91856200
C	5.79662100	2.88179800	-1.17184200
C	4.91880400	1.81005300	-1.06862800
O	-1.38271600	-1.15063100	0.18439500
O	1.36225500	1.16102600	-0.24985600
H	3.70265600	-0.98123200	-1.06009400
H	1.26779500	-2.09784400	-0.57494200
H	-3.72311700	0.99162600	0.99463400
H	-1.28825500	2.10823900	0.50948200
H	-2.13171000	-3.49173300	0.11135300
H	-3.69447100	-5.39202500	0.29610400
H	-6.06370200	-5.00625600	0.93429900
H	-6.84934400	-2.69236500	1.38575200
H	-5.29739000	-0.79664300	1.20360300
H	2.11124900	3.50212800	-0.17681300
H	3.67401000	5.40241900	-0.36156500
H	6.04324100	5.01665000	-0.99976100
H	6.82888200	2.70275900	-1.45121500
H	5.27692800	0.80703700	-1.26906600

4Ob compound

C	0.98060500	0.97266400	1.08562400
C	-0.01088500	0.04887000	0.68505100
C	0.01948600	-0.05697800	-0.67708200
C	1.56706200	1.38037800	-0.09822700
C	-1.55846100	-1.38848600	0.10619600
C	-0.97200300	-0.98077200	-1.07765500
C	-2.63472900	-2.32052400	0.39735500
C	2.64332900	2.31241700	-0.38938600
C	-3.04529200	-2.55924300	1.72024400
C	-4.07642900	-3.45321000	1.98979400
C	-4.71928300	-4.12679900	0.95251500
C	-4.31897200	-3.89663700	-0.36471800
C	-3.29021300	-3.00545500	-0.64158600
C	3.05389200	2.55113700	-1.71227500
C	4.08502800	3.44510500	-1.98182500
C	4.72788100	4.11869400	-0.94454700
C	4.32757100	3.88853200	0.37268600
C	3.29881300	2.99734900	0.64955500
H	1.24529000	1.30544800	2.07490300
H	-1.23668800	-1.31355600	-2.06693400
H	-2.55139700	-2.04038400	2.53143700
H	-4.37883300	-3.62395600	3.01700300
H	-5.52234400	-4.82269800	1.16591200
H	-4.81135400	-4.41452600	-1.18018400
H	-2.99363800	-2.83993600	-1.67069100
H	2.55999800	2.03227800	-2.52346800
H	4.38743100	3.61585100	-3.00903400
H	5.53094200	4.81459400	-1.15794300
H	4.81995200	4.40642200	1.18815200
H	3.00223900	2.83182900	1.67865900
O	-0.97018700	-0.75693300	1.19912600
O	0.97878900	0.74882500	-1.19115800

4Oc compound

C	-5.219165	-1.345732	0.115834
C	-6.315052	-2.214784	0.222334
C	-7.584796	-1.664846	0.348868
C	-7.780122	-0.272656	0.370966
C	-6.707595	0.610610	0.266773
C	-5.450205	0.041644	0.141410
O	-4.267161	0.720395	0.025880
C	-3.280277	-0.236793	-0.073477
C	-3.797262	-1.498155	-0.024902
C	-1.937815	0.251408	-0.205109
C	-1.420831	1.512769	-0.253683
C	0.001072	1.360346	-0.394419
C	0.232112	-0.027030	-0.419997
O	-0.950932	-0.705780	-0.304466
C	1.096959	2.229398	-0.500919
C	2.366703	1.679460	-0.627453
C	2.562029	0.287270	-0.649552
C	1.489502	-0.595996	-0.545359
H	-6.174977	-3.289414	0.206362
H	-8.444692	-2.319382	0.432504
H	-8.784371	0.122193	0.470961
H	-6.842978	1.684723	0.282283
H	-3.227366	-2.411173	-0.083058
H	-1.990727	2.425788	-0.195527
H	0.956884	3.304028	-0.484946
H	3.226599	2.333996	-0.711089
H	3.566278	-0.107578	-0.749548
H	1.624885	-1.670108	-0.560870

4Od compound

C	0.78416100	1.15978200	-1.07577800
C	-0.03474900	0.06117800	-0.67687500
C	0.02198200	-0.05116100	0.67823300
C	1.29053500	1.63652700	0.16374600
C	-1.30330200	-1.62651000	-0.16238800
C	-0.79692800	-1.14976500	1.07713600
C	-2.16117600	-2.70761900	-0.25645200
C	-2.52421700	-3.33309700	0.93589900
C	-2.03835900	-2.88227600	2.17353700
C	-1.17644000	-1.79501700	2.26039400
C	2.14840900	2.71763500	0.25781000
C	2.51145100	3.34311400	-0.93454100
C	2.02559200	2.89229300	-2.17217900
C	1.16367300	1.80503300	-2.25903600
H	-2.52882000	-3.04547100	-1.21726200
H	-3.19467000	-4.18375200	0.90428100
H	-2.34270100	-3.39382400	3.07920600
H	-0.80552700	-1.45265300	3.21863800
H	2.51605300	3.05548700	1.21862000
H	3.18190300	4.19376900	-0.90292300
H	2.32993500	3.40384100	-3.07784800
H	0.79276000	1.46267000	-3.21728000
O	-0.83949400	-0.88841200	-1.23867600
O	0.82672700	0.89842900	1.24003400

4Sa compound

C	2.62996200	1.05386600	-1.04464100
C	1.44349100	0.38631600	-0.65408300
C	0.39358000	1.23594900	-0.38408200
C	2.51505600	2.42384900	-1.07941800
C	-0.95140200	0.91903200	0.04181100
C	-3.13790300	-0.24636000	0.54817900
C	-3.10616700	1.07186800	0.93875900
C	-1.88207700	1.72639500	0.65750500
C	-4.22600100	-1.21821900	0.69220200
C	3.53411700	3.41974700	-1.42424200
C	-3.97323600	-2.59520200	0.80912600
C	-5.01738200	-3.50308400	0.95501100
C	-6.33763500	-3.05788300	0.99516100
C	-6.60359600	-1.69348100	0.88007900
C	-5.56296000	-0.78456200	0.72339700
C	3.50892600	4.71684100	-0.88523600
C	4.48966600	5.64671100	-1.21581200
C	5.52263500	5.30207500	-2.08592300
C	5.56031300	4.01779600	-2.62884000
C	4.57569100	3.08950100	-2.30886500
S	-1.61962600	-0.68134500	-0.21184600
S	0.88567400	2.89840300	-0.64137100
H	3.55777400	0.53917400	-1.25690700
H	1.37120900	-0.68798100	-0.54361300
H	-3.92998100	1.54972300	1.45235700
H	-1.67831400	2.75432600	0.92839900
H	-2.95027800	-2.95443200	0.80629900
H	-4.79748400	-4.56088000	1.04651000
H	-7.15034800	-3.76557200	1.11146300
H	-7.62729900	-1.33640100	0.89914700
H	-5.78566800	0.26899900	0.60229800
H	2.72689300	4.99171400	-0.18640200
H	4.45104400	6.64088400	-0.78478100
H	6.28773700	6.02627400	-2.34088300
H	6.35299700	3.74158400	-3.31527900
H	4.59878000	2.10602400	-2.76328900

4Sb compound

C	1.50108500	0.68835100	0.76029800
C	0.34132500	-0.11065500	0.59341400
C	-0.33803600	0.10610500	-0.59804500
C	1.71125200	1.52905700	-0.30681100
C	-1.70796300	-1.53360700	0.30218100
C	-1.49779500	-0.69290200	-0.76492800
C	-2.79407800	-2.50162300	0.48863400
C	2.79736600	2.49707300	-0.49326300
C	-3.26394500	-2.84046300	1.76833600
C	-4.30208300	-3.75283100	1.92903500
C	-4.90072600	-4.34201500	0.81672400
C	-4.44412700	-4.01515300	-0.46001600
C	-3.39899700	-3.11252300	-0.62354000
C	3.40228300	3.10797600	0.61891100
C	4.44741300	4.01060700	0.45538700
C	4.90401400	4.33746600	-0.82135200
C	4.30537400	3.74828000	-1.93366300
C	3.26723600	2.83591200	-1.77296500
H	2.17089300	0.63234300	1.60707200
H	-2.16760300	-0.63689300	-1.61170200
H	-2.82652200	-2.37036300	2.64187200
H	-4.65007100	-3.99663000	2.92657300
H	-5.71117100	-5.05063300	0.94279400
H	-4.89437100	-4.47590800	-1.33225000
H	-3.03101100	-2.89377400	-1.61906900
H	3.03429500	2.88922800	1.61444000
H	4.89765500	4.47136300	1.32762200
H	5.71445900	5.04608500	-0.94742200
H	4.65336400	3.99207800	-2.93120100
H	2.82981500	2.36581000	-2.64650100
S	-0.45111600	-1.34426500	1.53453800
S	0.45440600	1.33971400	-1.53916900

4Sc compound

C	-5.41557500	-1.12759900	0.18141400
C	-6.39884900	-2.11124500	0.39059600
C	-7.73225100	-1.74148600	0.46595500
C	-8.11290500	-0.39509100	0.33687100
C	-7.16222000	0.59715200	0.13124500
C	-5.81995900	0.22289700	0.05562000
S	-4.44043900	1.27493800	-0.20494800
C	-3.32688900	-0.10007300	-0.12272800
C	-3.99401900	-1.27590600	0.07685700
C	-1.90174700	0.11473700	-0.26294300
C	-1.20800800	1.29001000	-0.19267400
C	0.20646300	1.14193600	-0.36897700
C	0.57792400	-0.20782100	-0.57722700
S	-0.82630500	-1.25940300	-0.56722600
C	1.21197700	2.12519000	-0.35237700
C	2.53416400	1.75578000	-0.54136500
C	2.88171700	0.41012900	-0.74818300
C	1.90886100	-0.58173200	-0.76763200
H	-6.10870000	-3.15129100	0.49172700
H	-8.49222200	-2.49748100	0.62639900
H	-9.16082900	-0.12509900	0.39829900
H	-7.45861300	1.63486800	0.03280500
H	-3.49021000	-2.23015400	0.16493700
H	-1.68449200	2.24363500	-0.00364800
H	0.94760000	3.16467000	-0.19206700
H	3.31108000	2.51149100	-0.52988500
H	3.92127600	0.14043000	-0.89445400
H	2.17986900	-1.61888300	-0.92659000

4Sd compound

C	0.88287600	1.26081800	-0.98992200
C	0.04107800	0.14397400	-0.67070800
C	-0.04109500	-0.14396600	0.67070800
C	1.44045100	1.81020500	0.19317500
C	-1.44046700	-1.81019700	-0.19317500
C	-0.88289300	-1.26080900	0.98992200
C	-2.29755500	-2.90914400	-0.14802800
C	-2.60118400	-3.46517400	1.08936200
C	-2.05762900	-2.93312800	2.26886800
C	-1.20489300	-1.84021500	2.22712300
C	2.29753800	2.90915300	0.14802800
C	2.60116700	3.46518300	-1.08936200
C	2.05761200	2.93313600	-2.26886800
C	1.20487700	1.84022400	-2.22712300
H	-2.71882800	-3.32213100	-1.05718700
H	-3.26582400	-4.31967000	1.14127300
H	-2.30786400	-3.38237500	3.22288200
H	-0.78788200	-1.43333500	3.14152700
H	2.71881100	3.32214000	1.05718700
H	3.26580700	4.31967900	-1.14127300
H	2.30784700	3.38238300	-3.22288200
H	0.78786500	1.43334400	-3.14152700
S	-0.92151500	-0.94980300	-1.64837600
S	0.92149900	0.94981200	1.64837600

5Oa compound

C	0.54146700	1.20579100	0.45462800
C	-0.74991600	1.16715000	-0.04457200
C	-1.31645100	-0.03962700	-0.49258900
C	-0.53034100	-1.20244400	-0.41706200
C	0.76104100	-1.16380300	0.08213900
C	1.32757700	0.04297500	0.53015600
C	-2.66882000	-0.08979000	-1.01725800
C	2.67994600	0.09313800	1.05482400
C	-3.45594300	-1.10019600	-1.51049800
C	-4.69993700	-0.51703200	-1.87269000
C	-4.61443800	0.82122300	-1.58389900
C	3.46706900	1.10354400	1.54806600
C	4.71106200	0.52038000	1.91025700
C	4.62556400	-0.81787600	1.62146500
C	-5.53686000	1.93825000	-1.72157100
C	5.54798600	-1.93490200	1.75913500
C	-5.16610100	3.23717100	-1.33610100
C	-6.05674700	4.29724600	-1.47283100
C	-7.33192200	4.08675700	-1.99489600
C	-7.71015600	2.79985900	-2.38082700
C	-6.82532300	1.73726900	-2.24668900
C	5.17722900	-3.23382200	1.37366100
C	6.06787500	-4.29389700	1.51039000
C	7.34304900	-4.08340900	2.03245800
C	7.72128100	-2.79651100	2.41839400
C	6.83644800	-1.73392100	2.28425700
O	-3.37556300	1.08310700	-1.06191200
O	3.38668900	-1.07975900	1.09947800
H	0.94609000	2.15318200	0.79115300
H	-1.33339800	2.07750200	-0.09144500
H	-0.93496500	-2.14983400	-0.75358700
H	1.34452300	-2.07415400	0.12901100
H	-3.18010700	-2.13806100	-1.60412600
H	-5.55073200	-1.02707700	-2.29459500
H	3.19123200	2.14140900	1.64169500
H	5.56185800	1.03042500	2.33216300
H	-4.17764300	3.40887400	-0.92997100
H	-5.75230500	5.29287900	-1.16975100
H	-8.02386100	4.91435000	-2.10038800
H	-8.69954000	2.62403100	-2.78810900
H	-7.13538600	0.74442400	-2.55101100
H	4.18877200	-3.40552500	0.96752900
H	5.76343500	-5.28952900	1.20730600
H	8.03498900	-4.91100200	2.13795000
H	8.71066500	-2.62068400	2.82567800
H	7.14651000	-0.74107700	2.58858200

5Ob compound

C	0.48079900	-1.29852600	0.18557000
C	-0.26913700	-0.14179700	-0.06940300
C	0.38343800	1.10682100	-0.22556800
C	1.74911100	1.29949400	-0.14658400
C	2.49904700	0.14276500	0.10838900
C	1.84647200	-1.10585200	0.26455400
C	3.89690400	-0.13867200	0.26947400
C	4.01487000	-1.47845400	0.50366500
O	2.77381400	-2.08459800	0.50419600
C	-1.66699400	0.13964100	-0.23048900
C	-1.78495900	1.47942300	-0.46468000
O	-0.54390400	2.08556600	-0.46521100
C	5.16161000	-2.34479300	0.74267900
C	-2.93170000	2.34576100	-0.70369500
C	4.98941300	-3.72095500	0.96231300
C	6.08926000	-4.54256000	1.19032000
C	7.37724100	-4.01073400	1.20380300
C	7.55842500	-2.64369100	0.98637000
C	6.46466500	-1.81853200	0.75823900
C	-2.75950200	3.72192400	-0.92332600
C	-3.85934900	4.54352800	-1.15133500
C	-5.14733100	4.01170200	-1.16482100
C	-5.32851400	2.64465800	-0.94739000
C	-4.23475500	1.81950000	-0.71925800
H	0.03012700	-2.27442400	0.31242400
H	2.19978300	2.27539300	-0.27343800
H	4.70755000	0.57008500	0.21698900
H	-2.47764000	-0.56911600	-0.17800400
H	3.99108500	-4.13849800	0.95288000
H	5.93823200	-5.60305400	1.35814700
H	8.23229100	-4.65277100	1.38162200
H	8.55644800	-2.22015200	0.99481300
H	6.62203100	-0.75950300	0.59105300
H	-1.76117500	4.13946800	-0.91389200
H	-3.70832200	5.60402300	-1.31916100
H	-6.00238100	4.65373900	-1.34264100
H	-6.32653700	2.22111900	-0.95583600
H	-4.39212100	0.76047000	-0.55207400

5Oc compound

C	-5.53528800	-1.64671800	1.38236000
C	-5.65808100	-0.24694300	1.33746100
C	-6.82579600	0.43345800	1.64552400
C	-7.91907100	-0.34651900	2.01651100
C	-7.83025600	-1.74871700	2.07173400
C	-6.64954300	-2.41122200	1.75870700
C	-4.18042700	-1.92382200	0.99513700
C	-3.58298000	-0.72059700	0.74730200
O	-4.47409600	0.31618300	0.95224900
C	-2.24139300	-0.34934100	0.32662700
C	-1.88667300	0.99875500	0.14452600
C	-0.60732300	1.34806100	-0.25604800
C	0.37131900	0.36846700	-0.49180200
C	0.01659900	-0.97962800	-0.30970000
C	-1.26275100	-1.32893400	0.09087400
C	1.71290700	0.73972400	-0.91247600
O	2.60402100	-0.29705700	-1.11742800
C	3.78800700	0.26606900	-1.50263800
C	3.66521500	1.66584500	-1.54753000
C	2.31035500	1.94294900	-1.16030500
C	4.95572000	-0.41433200	-1.81070500
C	6.04899600	0.36564500	-2.18168900
C	5.96018300	1.76784400	-2.23690500
C	4.77947100	2.43034900	-1.92387400
H	-6.87967100	1.51390100	1.59865200
H	-8.85567600	0.13762000	2.26720900
H	-8.70273300	-2.32122900	2.36490800
H	-6.59200200	-3.49268100	1.80456900
H	-3.71488900	-2.89279400	0.91305600
H	-2.62483000	1.77014300	0.32057300
H	-0.36571100	2.39615400	-0.38729000
H	0.75475600	-1.75101700	-0.48574800
H	-1.50436300	-2.37702700	0.22211500
H	1.84481900	2.91192100	-1.07821900
H	5.00959400	-1.49477500	-1.76383900
H	6.98560000	-0.11849500	-2.43239000
H	6.83266100	2.34035600	-2.53007600
H	4.72193100	3.51180800	-1.96973100

5Od compound

C	0.76577300	1.30976000	0.31492500
C	1.60357200	0.20720600	0.11949400
C	1.05148800	-1.06531200	-0.15833300
C	-0.30344000	-1.32152000	-0.25707200
C	-1.14123900	-0.21896600	-0.06164100
C	-0.58915500	1.05355200	0.21618600
C	-2.57729600	-0.02008300	-0.07056800
C	-2.77180000	1.34539400	0.20052000
O	-1.57703000	2.00179300	0.37512300
C	3.03963000	0.00832300	0.12842100
C	3.23413300	-1.35715400	-0.14266700
O	2.03936300	-2.01355300	-0.31726900
C	-3.69347200	-0.83716500	-0.27522400
C	-4.96020400	-0.26575200	-0.20262200
C	-5.12233500	1.10115300	0.06987600
C	-4.02367500	1.93418300	0.27719700
C	4.15580500	0.82540500	0.33307700
C	5.42253700	0.25399200	0.26047600
C	5.58466800	-1.11291300	-0.01202300
C	4.48600800	-1.94594300	-0.21934400
H	1.14218300	2.30162400	0.52965800
H	-0.67985000	-2.31338400	-0.47180500
H	-3.57723900	-1.89406900	-0.48622700
H	-5.83661900	-0.88378700	-0.35854100
H	-6.12089800	1.51948800	0.12059700
H	-4.13518300	2.99021800	0.48821100
H	4.03957200	1.88230900	0.54408000
H	6.29895200	0.87202700	0.41639400
H	6.58323200	-1.53124800	-0.06274400
H	4.59751600	-3.00197800	-0.43035800

5Sa compound

C	0.90828100	1.40940600	-0.21299400
C	-0.31021300	1.47437600	-0.87151900
C	-0.97010500	0.31122600	-1.30398700
C	-0.35002900	-0.92181000	-1.03778800
C	0.86846500	-0.98678000	-0.37926400
C	1.52835600	0.17637000	0.05320500
C	-2.24874300	0.36448600	-2.01370400
C	2.80699500	0.12311000	0.76292200
C	-2.77880700	-0.54566200	-2.89925200
C	-4.05021300	-0.17917300	-3.40644600
C	-4.51951600	1.01865100	-2.92031400
C	3.33705900	1.03325800	1.64847000
C	4.60846500	0.66676900	2.15566400
C	5.07776800	-0.53105500	1.66953200
C	-5.78190800	1.69930200	-3.22711900
C	6.34015900	-1.21170600	1.97633700
C	-5.89823300	3.09790600	-3.16714400
C	-7.10065200	3.72829200	-3.47154200
C	-8.21295300	2.97850200	-3.85045000
C	-8.11214400	1.58885600	-3.91423000
C	-6.91477700	0.95524800	-3.59991100
C	6.45648500	-2.61031000	1.91636200
C	7.65890300	-3.24069600	2.22076000
C	8.77120400	-2.49090600	2.59966800
C	8.67039600	-1.10126000	2.66344800
C	7.47302800	-0.46765200	2.34912900
S	-3.36294100	1.69847700	-1.79545900
S	3.92119300	-1.21088100	0.54467700
H	1.40275100	2.33000600	0.07343200
H	-0.74258200	2.44601900	-1.08252900
H	-0.84450000	-1.84241000	-1.32421400
H	1.30083300	-1.95842200	-0.16825300
H	-2.25086900	-1.43799800	-3.20906700
H	-4.58817000	-0.76363800	-4.14133800
H	2.80912000	1.92559400	1.95828500
H	5.14642100	1.25123400	2.89055600
H	-5.03460600	3.69630400	-2.89966700
H	-7.16557200	4.80946200	-3.42116600
H	-9.14854500	3.47053700	-4.09013200
H	-8.97372300	0.99441400	-4.19739700
H	-6.85923800	-0.12674800	-3.62204900
H	5.59285800	-3.20870700	1.64888500
H	7.72382300	-4.32186600	2.17038400
H	9.70679700	-2.98294100	2.83935000
H	9.53197500	-0.50681800	2.94661600
H	7.41748900	0.61434400	2.37126700

5Sb compound

C	-0.97650000	-0.09389300	-0.96827600
C	-1.34104100	-0.10225800	0.40914300
C	-0.34198500	-0.00349500	1.38730600
C	0.97649500	0.09388800	0.96825500
C	1.34103600	0.10225300	-0.40916400
C	0.34197900	0.00348900	-1.38732700
C	3.46718800	0.28208700	0.57767100
C	2.76057800	0.20783500	-0.58631900
C	-3.46719400	-0.28209200	-0.57769300
C	-2.76058300	-0.20784000	0.58629800
C	4.92053400	0.39689900	0.74957300
C	-4.92053900	-0.39690400	-0.74959400
C	5.56639100	-0.11638800	1.88580600
C	6.94691100	-0.01460900	2.02839100
C	7.71308900	0.59977600	1.03957200
C	7.08396600	1.11817000	-0.09233200
C	5.70391600	1.02415500	-0.23419200
C	-5.56639700	0.11638300	-1.88582700
C	-6.94691700	0.01460400	-2.02841300
C	-7.71309400	-0.59978100	-1.03959300
C	-7.08397200	-1.11817500	0.09231100
C	-5.70392200	-1.02416000	0.23417100
H	-0.60174400	-0.00620900	2.43971100
H	0.60173800	0.00620400	-2.43973200
H	3.23404300	0.19751400	-1.55963600
H	-3.23404800	-0.19751900	1.55961500
H	4.98548600	-0.61581600	2.65287700
H	7.42510700	-0.42196200	2.91208100
H	8.78837100	0.67869900	1.15132600
H	7.66909700	1.60914600	-0.86193900
H	5.22340800	1.45855500	-1.10285800
H	-4.98549100	0.61581100	-2.65289800
H	-7.42511200	0.42195700	-2.91210200
H	-8.78837700	-0.67870400	-1.15134700
H	-7.66910300	-1.60915100	0.86191800
H	-5.22341300	-1.45856000	1.10283700
S	2.39960600	0.22987100	1.99100400
S	-2.39961200	-0.22987600	-1.99102500

5Sc compound

C	-5.62407500	-1.29408400	1.63748600
C	-6.17686100	-0.11565200	1.08199400
C	-7.53008000	0.19766200	1.22249700
C	-8.34002400	-0.67964100	1.93228900
C	-7.80979300	-1.85294600	2.49573700
C	-6.46655600	-2.16271100	2.35463400
C	-4.21957300	-1.40694700	1.37077900
C	-3.70510600	-0.37242900	0.64341800
S	-4.95428200	0.81491700	0.23762700
C	-2.32134400	-0.17592100	0.20159400
C	-1.79505700	1.10509400	-0.03340300
C	-0.48116500	1.27880900	-0.44218200
C	0.37528300	0.18013400	-0.62221300
C	-0.15353700	-1.10137300	-0.39575800
C	-1.47145300	-1.27586200	-0.00046300
C	1.76910400	0.37869000	-1.03020300
S	2.63117000	-0.88267700	-1.92498500
C	4.08664200	0.09273100	-1.98679000
C	3.88980300	1.33929000	-1.34632600
C	2.56438900	1.46713900	-0.81394700
C	5.30650300	-0.24595100	-2.57529700
C	6.34468100	0.67514000	-2.51824200
C	6.17127000	1.91668700	-1.88281800
C	4.95953100	2.25150100	-1.29995100
H	-7.94074600	1.10272900	0.79038500
H	-9.39343500	-0.45460000	2.05291100
H	-8.46143500	-2.52156500	3.04643900
H	-6.06153000	-3.06890300	2.79179900
H	-3.61330900	-2.22383800	1.74045200
H	-2.42150400	1.97795700	0.11139300
H	-0.11670300	2.28008300	-0.63828300
H	0.47746400	-1.97334900	-0.52532400
H	-1.85226900	-2.28030400	0.14065400
H	2.23267100	2.33657000	-0.26114500
H	5.44303800	-1.20347000	-3.06420400
H	7.29983600	0.43140300	-2.96894900
H	6.99660700	2.61861100	-1.84990200
H	4.83045000	3.21047800	-0.81000700

5Sd compound

C	1.27510000	0.05301300	0.58811700
C	2.67553100	0.05312600	0.97727300
C	3.53031500	-0.24575400	-0.10485100
C	1.10373100	-0.24775600	-0.78724300
C	-0.15059500	-0.30309700	-1.37990900
C	-1.27510000	-0.05301300	-0.58811700
C	-1.10373100	0.24775600	0.78724300
C	0.15059500	0.30309700	1.37990900
C	3.24166400	0.30249600	2.23508700
C	4.61975900	0.25228000	2.39567600
C	5.45274500	-0.04637800	1.30846200
C	4.91544000	-0.29751000	0.05091000
C	-2.67553100	-0.05312600	-0.97727300
C	-3.53031500	0.24575400	0.10485100
C	-3.24166400	-0.30249600	-2.23508700
C	-4.61975900	-0.25228000	-2.39567600
C	-5.45274500	0.04637800	-1.30846200
C	-4.91544000	0.29751000	-0.05091000
H	-0.25787400	-0.53491400	-2.43305800
H	0.25787400	0.53491400	2.43305800
H	2.60527200	0.53429200	3.08187400
H	5.05583600	0.44533500	3.36885500
H	6.52722300	-0.08254000	1.44682800
H	5.56061600	-0.52823700	-0.78866900
H	-2.60527200	-0.53429200	-3.08187400
H	-5.05583600	-0.44533500	-3.36885500
H	-6.52722300	0.08254000	-1.44682800
H	-5.56061600	0.52823700	0.78866900
S	2.64496100	-0.53022500	-1.60641600
S	-2.64496100	0.53022500	1.60641600

5.2 Cationic ground state

4Oa compound

C	2.77994500	-0.45663500	-0.77792800
C	1.54325700	-1.04497600	-0.53347400
C	0.66587800	-0.00702800	-0.20247300
C	2.63051700	0.92282000	-0.59131200
C	-0.68633900	0.01742300	0.13701200
C	-2.65097800	-0.91242600	0.52585100
C	-2.80040700	0.46702900	0.71246700
C	-1.56371800	1.05537100	0.46801300
C	-3.56223000	-2.01226000	0.63390100
C	3.54176800	2.02265500	-0.69936200
C	-3.13393500	-3.33240900	0.38298700
C	-4.02908100	-4.38330300	0.49244000
C	-5.35737400	-4.13966100	0.85126200
C	-5.79171000	-2.83544500	1.10195900
C	-4.90583100	-1.77708300	0.99558300
C	3.11347400	3.34280300	-0.44844800
C	4.00862000	4.39369800	-0.55790100
C	5.33691300	4.15005500	-0.91672300
C	5.77124800	2.84583900	-1.16742000
C	4.88537000	1.78747700	-1.06104400
O	-1.35924900	-1.17338300	0.17569000
O	1.33878800	1.18377700	-0.24115100
H	3.69009700	-0.95962200	-1.05914500
H	1.28556100	-2.09038900	-0.58241900
H	-3.71055800	0.97001600	0.99368400
H	-1.30602200	2.10078400	0.51695800
H	-2.10508600	-3.51767000	0.10544300
H	-3.69775600	-5.39588100	0.29926000
H	-6.05362400	-4.96513500	0.93554100
H	-6.82167200	-2.65062100	1.37977500
H	-5.24925300	-0.76932500	1.19132600
H	2.08462500	3.52806400	-0.17090400
H	3.67729500	5.40627500	-0.36472100
H	6.03316300	4.97553000	-1.00100200
H	6.80121100	2.66101600	-1.44523600
H	5.22879200	0.77971900	-1.25678700

4Ob compound

C	0.96623900	0.95908700	1.08805400
C	-0.00481500	0.05544400	0.70239400
C	0.01341500	-0.06355000	-0.69442500
C	1.56040900	1.37164700	-0.12563700
C	-1.55180900	-1.37975300	0.13360600
C	-0.95763900	-0.96719400	-1.08008500
C	-2.60823800	-2.29552300	0.41074700
C	2.61683800	2.28741700	-0.40277800
C	-3.02096400	-2.53513400	1.74147800
C	-4.04783100	-3.42691200	1.99517100
C	-4.67826100	-4.09156800	0.93915400
C	-4.27797000	-3.86203100	-0.38141700
C	-3.25336800	-2.97367000	-0.64959600
C	3.02956400	2.52702700	-1.73350900
C	4.05643200	3.41880500	-1.98720200
C	4.68686100	4.08346200	-0.93118500
C	4.28657000	3.85392500	0.38938600
C	3.26196800	2.96556400	0.65756400
H	1.23958900	1.29824400	2.07235800
H	-1.23098900	-1.30635000	-2.06439000
H	-2.53040900	-2.01872600	2.55513300
H	-4.36287700	-3.60946300	3.01474300
H	-5.48164200	-4.78863400	1.14412800
H	-4.77015400	-4.37984900	-1.19478700
H	-2.94903200	-2.80109500	-1.67391500
H	2.53900900	2.01062000	-2.54716400
H	4.37147700	3.60135600	-3.00677400
H	5.49024200	4.78052800	-1.13615900
H	4.77875400	4.37174300	1.20275600
H	2.95763200	2.79298900	1.68188400
O	-0.95727000	-0.74421200	1.21931000
O	0.96587000	0.73610600	-1.21134200

4Oc compound

C	-5.20223000	-1.33780200	0.11419500
C	-6.30130300	-2.22365700	0.22096000
C	-7.55863400	-1.67472900	0.34624500
C	-7.74851000	-0.27209600	0.36784300
C	-6.68604900	0.62825300	0.26470000
C	-5.43511400	0.06453300	0.13999400
O	-4.24915400	0.74055600	0.02417000
C	-3.27004300	-0.21048100	-0.07442100
C	-3.81208100	-1.49952700	-0.02341800
C	-1.94805000	0.22509600	-0.20416400
C	-1.40601200	1.51414100	-0.25516700
C	-0.01586200	1.35241600	-0.39278100
C	0.21702100	-0.04991800	-0.41858000
O	-0.96893900	-0.72594100	-0.30275600
C	1.08321000	2.23827100	-0.49954600
C	2.34054100	1.68934300	-0.62483100
C	2.53041700	0.28671000	-0.64642900
C	1.46795600	-0.61363900	-0.54328500
H	-6.15081100	-3.29535600	0.20395700
H	-8.42359500	-2.31983800	0.43037600
H	-8.75436400	0.11709500	0.46797600
H	-6.83513500	1.69926300	0.28156300
H	-3.24307100	-2.41404600	-0.08145900
H	-1.97502100	2.42866100	-0.19712600
H	0.93271800	3.30997000	-0.48254300
H	3.20550300	2.33445200	-0.70896300
H	3.53627100	-0.10248100	-0.74656200
H	1.61704200	-1.68464900	-0.56014900

4Od compound

C	0.77623400	1.14979500	-1.07678800
C	-0.03272700	0.06753000	-0.70458700
C	0.01996000	-0.05751300	0.70594500
C	1.28407400	1.62707700	0.17252400
C	-1.29684100	-1.61706000	-0.17116600
C	-0.78900100	-1.13977800	1.07814600
C	-2.14572100	-2.68536200	-0.27508800
C	-2.50530700	-3.30856500	0.93275400
C	-2.02585700	-2.86718000	2.17970200
C	-1.16817700	-1.78631900	2.27395900
C	2.13295500	2.69537800	0.27644700
C	2.49254100	3.31858200	-0.93139500
C	2.01309100	2.87719600	-2.17834300
C	1.15541000	1.79633500	-2.27260100
H	-2.51766100	-3.02938200	-1.23083000
H	-3.17562800	-4.15857700	0.89762000
H	-2.33679900	-3.38600800	3.07698300
H	-0.79457100	-1.44002400	3.22859900
H	2.50489500	3.03939900	1.23218800
H	3.16286100	4.16859300	-0.89626100
H	2.32403200	3.39602500	-3.07562500
H	0.78180500	1.45004100	-3.22724000
O	-0.81905800	-0.86007100	-1.25536800
O	0.80629100	0.87008800	1.25672700

4Sa compound

C	2.51439300	1.04005300	-1.29970600
C	1.33776800	0.39100100	-0.96633600
C	0.32173000	1.25833700	-0.52519600
C	2.46413700	2.43336400	-1.12913700
C	-0.98134900	0.93142700	-0.11432900
C	-3.12775400	-0.24206700	0.47818000
C	-3.16750400	1.14755000	0.67895000
C	-1.98735600	1.79529700	0.35565800
C	-4.17572100	-1.20376500	0.72096400
C	3.51072000	3.39564900	-1.37551900
C	-3.91860200	-2.59092200	0.68938600
C	-4.93373500	-3.50218900	0.92434400
C	-6.22885300	-3.05311900	1.19452900
C	-6.50149400	-1.68404700	1.22790900
C	-5.49016700	-0.76671700	0.99568900
C	3.39100200	4.73423400	-0.94517200
C	4.40308300	5.64673900	-1.18829900
C	5.55718800	5.24769500	-1.86711400
C	5.69163000	3.92748700	-2.30162500
C	4.68374900	3.00877700	-2.06005100
S	-1.56839200	-0.72453500	-0.14268900
S	0.89097500	2.92057800	-0.54801000
H	3.40102700	0.52514900	-1.63862000
H	1.20492900	-0.68098600	-1.02496100
H	-4.03538300	1.65583000	1.07208800
H	-1.83826400	2.86155400	0.46104700
H	-2.91553600	-2.95318600	0.49692800
H	-4.72079200	-4.56355800	0.90261700
H	-7.02186200	-3.76765100	1.37810500
H	-7.50632300	-1.33587700	1.43170100
H	-5.72124100	0.29008000	1.00855900
H	2.50842300	5.05380600	-0.40356400
H	4.30012500	6.66921900	-0.84733600
H	6.34804400	5.96311100	-2.05643900
H	6.58354600	3.61936500	-2.83264200
H	4.79604900	1.99396600	-2.41772000

4Sb compound

C	1.25738300	0.93611000	0.87728500
C	0.20152700	0.06366100	0.67727800
C	-0.19824000	-0.06820800	-0.68190600
C	1.70727700	1.50840200	-0.32725900
C	-1.70398900	-1.51295000	0.32263100
C	-1.25409600	-0.94065700	-0.88191400
C	-2.77581600	-2.45643300	0.49448200
C	2.77910500	2.45188300	-0.49911100
C	-3.15355800	-2.90633200	1.78048100
C	-4.18522700	-3.81403700	1.93607800
C	-4.86682000	-4.29764000	0.81554400
C	-4.50792000	-3.86552200	-0.46421300
C	-3.47762600	-2.95715600	-0.62774000
C	3.48089600	2.95262800	0.62311300
C	4.51119100	3.86099300	0.45958600
C	4.87011000	4.29309000	-0.82017300
C	4.18853500	3.80946500	-1.94070900
C	3.15686600	2.90176100	-1.78511200
H	1.69750100	1.15767300	1.83728300
H	-1.69421200	-1.16222200	-1.84191200
H	-2.63788600	-2.53823200	2.65939800
H	-4.46428500	-4.14830600	2.92725900
H	-5.67441600	-5.00868700	0.93945500
H	-5.03559100	-4.24222400	-1.33132300
H	-3.21096300	-2.63773600	-1.62603600
H	3.21421700	2.63322700	1.62141100
H	5.03884700	4.23771300	1.32669700
H	5.67770600	5.00413600	-0.94408400
H	4.46760900	4.14371600	-2.93189200
H	2.64120900	2.53364200	-2.66403000
S	-0.77343000	-0.93667100	1.71490000
S	0.77671800	0.93212300	-1.71952900

4Sc compound

C	-5.41251100	-1.14906300	0.13552600
C	-6.40578100	-2.12624400	0.23155100
C	-7.74694500	-1.73675000	0.36467400
C	-8.10438800	-0.38996900	0.40268900
C	-7.12976700	0.60725500	0.30858600
C	-5.79647900	0.21230700	0.17621100
S	-4.41139600	1.26062000	0.04149200
C	-3.31839500	-0.11125800	-0.06935600
C	-3.99202600	-1.30313000	-0.00514600
C	-1.89969800	0.12587300	-0.20923000
C	-1.22606600	1.31774500	-0.27343600
C	0.19441900	1.16367800	-0.41410900
C	0.57838600	-0.19769200	-0.45480000
S	-0.80670100	-1.24600500	-0.32008500
C	1.18768900	2.14085800	-0.51013100
C	2.52885300	1.75136300	-0.64325700
C	2.88629400	0.40458200	-0.68127900
C	1.91167400	-0.59264100	-0.58717900
H	-6.14349900	-3.17697400	0.20347900
H	-8.51455000	-2.49667700	0.43882200
H	-9.14448100	-0.10893100	0.50588100
H	-7.40469000	1.65419500	0.33786400
H	-3.50348500	-2.26725700	-0.05536600
H	-1.71460700	2.28187200	-0.22321000
H	0.92540900	3.19158900	-0.48205500
H	3.29645800	2.51129000	-0.71740300
H	3.92638700	0.12354400	-0.78447300
H	2.18659500	-1.63958200	-0.61646100

4Sd compound

C	0.87621900	1.25389500	-1.00158100
C	0.03959000	0.14592500	-0.69904000
C	-0.03960700	-0.14591700	0.69904000
C	1.43046900	1.79837300	0.18648000
C	-1.43048600	-1.79836500	-0.18648000
C	-0.87623600	-1.25388700	1.00158100
C	-2.27971500	-2.88494700	-0.15851900
C	-2.58684400	-3.44718400	1.09152900
C	-2.05319600	-2.92820400	2.27414100
C	-1.19859500	-1.83409900	2.24120400
C	2.27969900	2.88495500	0.15851900
C	2.58682700	3.44719200	-1.09152900
C	2.05318000	2.92821300	-2.27414100
C	1.19857800	1.83410700	-2.24120400
H	-2.70173600	-3.29920700	-1.06535700
H	-3.25193900	-4.30085000	1.13303300
H	-2.30848200	-3.38311400	3.22229700
H	-0.78372800	-1.43012800	3.15682200
H	2.70171900	3.29921500	1.06535700
H	3.25192200	4.30085800	-1.13303300
H	2.30846600	3.38312200	-3.22229700
H	0.78371200	1.43013600	-3.15682200
S	-0.90168300	-0.92382300	-1.65388400
S	0.90166600	0.92383100	1.65388400

5Oa compound

C	0.54776900	1.21318900	0.45624600
C	-0.73227700	1.18987100	-0.03516500
C	-1.31196300	-0.02361900	-0.48728300
C	-0.53664300	-1.20984100	-0.41868100
C	0.74340300	-1.18652300	0.07273000
C	1.32308900	0.02696700	0.52484800
C	-2.63554200	-0.05701700	-0.99732800
C	2.64666800	0.06036500	1.03489400
C	-3.44069900	-1.07927200	-1.49877800
C	-4.66313800	-0.50493900	-1.85458200
C	-4.57664300	0.85481900	-1.56235900
C	3.45182500	1.08262000	1.53634300
C	4.67426400	0.50828600	1.89214700
C	4.58776900	-0.85147100	1.59992400
C	-5.50089500	1.94638000	-1.70607700
C	5.51202100	-1.94303200	1.74364200
C	-5.14088000	3.25236900	-1.32085300
C	-6.04398700	4.29380000	-1.46614900
C	-7.31397000	4.05379800	-1.99457800
C	-7.68034600	2.76218600	-2.37945300
C	-6.78496500	1.71454600	-2.23829000
C	5.15200600	-3.24902100	1.35841800
C	6.05511300	-4.29045300	1.50371400
C	7.32509600	-4.05045000	2.03214300
C	7.69147200	-2.75883800	2.41701800
C	6.79609100	-1.71119800	2.27585500
O	-3.34496900	1.11608500	-1.04365900
O	3.35609500	-1.11273700	1.08122400
H	0.96880500	2.15083100	0.79536500
H	-1.31197100	2.10140600	-0.08173600
H	-0.95767900	-2.14748300	-0.75780000
H	1.32309700	-2.09805800	0.11930100
H	-3.16430900	-2.11681600	-1.59145300
H	-5.51653300	-1.00953600	-2.27568100
H	3.17543500	2.12016300	1.62901900
H	5.52765900	1.01288300	2.31324700
H	-4.15663700	3.43637500	-0.91173700
H	-5.76222500	5.29618600	-1.16843900
H	-8.01658000	4.87056300	-2.10637600
H	-8.66544500	2.57707200	-2.78911100
H	-7.07702000	0.71636200	-2.53903700
H	4.16776300	-3.43302700	0.94930200
H	5.77335100	-5.29283800	1.20600400
H	8.02770600	-4.86721500	2.14394200
H	8.67657100	-2.57372300	2.82667700
H	7.08814500	-0.71301400	2.57660200

5Ob compound

C	0.54776900	1.21318900	0.45624600
C	-0.73227700	1.18987100	-0.03516500
C	-1.31196300	-0.02361900	-0.48728300
C	-0.53664300	-1.20984100	-0.41868100
C	0.74340300	-1.18652300	0.07273000
C	1.32308900	0.02696700	0.52484800
C	-2.63554200	-0.05701700	-0.99732800
C	2.64666800	0.06036500	1.03489400
C	-3.44069900	-1.07927200	-1.49877800
C	-4.66313800	-0.50493900	-1.85458200
C	-4.57664300	0.85481900	-1.56235900
C	3.45182500	1.08262000	1.53634300
C	4.67426400	0.50828600	1.89214700
C	4.58776900	-0.85147100	1.59992400
C	-5.50089500	1.94638000	-1.70607700
C	5.51202100	-1.94303200	1.74364200
C	-5.14088000	3.25236900	-1.32085300
C	-6.04398700	4.29380000	-1.46614900
C	-7.31397000	4.05379800	-1.99457800
C	-7.68034600	2.76218600	-2.37945300
C	-6.78496500	1.71454600	-2.23829000
C	5.15200600	-3.24902100	1.35841800
C	6.05511300	-4.29045300	1.50371400
C	7.32509600	-4.05045000	2.03214300
C	7.69147200	-2.75883800	2.41701800
C	6.79609100	-1.71119800	2.27585500
O	-3.34496900	1.11608500	-1.04365900
O	3.35609500	-1.11273700	1.08122400
H	0.96880500	2.15083100	0.79536500
H	-1.31197100	2.10140600	-0.08173600
H	-0.95767900	-2.14748300	-0.75780000
H	1.32309700	-2.09805800	0.11930100
H	-3.16430900	-2.11681600	-1.59145300
H	-5.51653300	-1.00953600	-2.27568100
H	3.17543500	2.12016300	1.62901900
H	5.52765900	1.01288300	2.31324700
H	-4.15663700	3.43637500	-0.91173700
H	-5.76222500	5.29618600	-1.16843900
H	-8.01658000	4.87056300	-2.10637600
H	-8.66544500	2.57707200	-2.78911100
H	-7.07702000	0.71636200	-2.53903700
H	4.16776300	-3.43302700	0.94930200
H	5.77335100	-5.29283800	1.20600400
H	8.02770600	-4.86721500	2.14394200
H	8.67657100	-2.57372300	2.82667700
H	7.08814500	-0.71301400	2.57660200

5Oc compound

C	-5.49898000	-1.62725600	1.37015400
C	-5.63211600	-0.21776000	1.32826500
C	-6.80027000	0.44918700	1.63759500
C	-7.88010300	-0.35327900	2.00569700
C	-7.78550500	-1.76218400	2.05905900
C	-6.60944000	-2.41370000	1.74643800
C	-4.16546100	-1.89899400	0.98877300
C	-3.55700600	-0.67196400	0.73667700
O	-4.44976000	0.35195200	0.94324300
C	-2.24000000	-0.32892400	0.32501300
C	-1.87204200	1.02856100	0.13734000
C	-0.60119600	1.35661100	-0.25947600
C	0.36992500	0.34805000	-0.49019100
C	0.00196600	-1.00943500	-0.30251800
C	-1.26887900	-1.33748500	0.09429800
C	1.68693100	0.69109000	-0.90185300
O	2.57968300	-0.33282600	-1.10842700
C	3.76204100	0.23688600	-1.49344500
C	3.62890800	1.64638200	-1.53532200
C	2.29539000	1.91812000	-1.15394000
C	4.93019300	-0.43006100	-1.80277900
C	6.01002900	0.37240500	-2.17087400
C	5.91543400	1.78131100	-2.22422500
C	4.73937000	2.43282700	-1.91159800
H	-6.87221000	1.52759700	1.59662500
H	-8.82147400	0.11871100	2.25879300
H	-8.65669500	-2.33415000	2.35167800
H	-6.53598500	-3.49298700	1.78702300
H	-3.69652500	-2.86612600	0.90510500
H	-2.60656200	1.80261400	0.31122800
H	-0.34038000	2.39775500	-0.39701400
H	0.73648700	-1.78348800	-0.47640700
H	-1.52969500	-2.37862900	0.23183600
H	1.82645500	2.88525300	-1.07026400
H	5.00213000	-1.50847200	-1.76181900
H	6.95139800	-0.09958600	-2.42397400
H	6.78662500	2.35327600	-2.51683800
H	4.66591800	3.51211400	-1.95217400

5Od compound

C	0.77440000	1.32686700	0.31871700
C	1.60104900	0.19796300	0.11751000
C	1.02885200	-1.09627600	-0.16543600
C	-0.31206700	-1.33862600	-0.26086400
C	-1.13871600	-0.20972200	-0.05965600
C	-0.56651900	1.08451600	0.22328900
C	-2.54169100	-0.01181400	-0.06762700
C	-2.74439700	1.36922800	0.20633800
O	-1.55048000	2.02313600	0.38041200
C	3.00402400	0.00005400	0.12548000
C	3.20673000	-1.38098800	-0.14848500
O	2.01281300	-2.03489500	-0.32255900
C	-3.65845800	-0.85060100	-0.27672200
C	-4.91459500	-0.28644400	-0.20526300
C	-5.07812200	1.09103200	0.06931900
C	-3.99224700	1.94613900	0.28071300
C	4.12079100	0.83884100	0.33457500
C	5.37692900	0.27468300	0.26311700
C	5.54045600	-1.10279300	-0.01146600
C	4.45458000	-1.95790000	-0.22286000
H	1.17093000	2.30994300	0.53236800
H	-0.70859700	-2.32170200	-0.47451500
H	-3.52860700	-1.90465300	-0.48665900
H	-5.79332900	-0.89876700	-0.36011500
H	-6.08043800	1.49906300	0.11778600
H	-4.12213800	2.99912200	0.49046400
H	3.99094100	1.89289300	0.54451200
H	6.25566300	0.88700600	0.41796800
H	6.54277100	-1.51082400	-0.05993300
H	4.58447000	-3.01088200	-0.43261000

5Sa compound

C	0.76265100	1.37697800	0.02689700
C	-0.45931200	1.42307700	-0.59320800
C	-0.99044400	0.29348400	-1.26888200
C	-0.20440000	-0.88938200	-1.27767800
C	1.01756400	-0.93548100	-0.65757300
C	1.54869500	0.19411200	0.01810000
C	-2.26399300	0.33310100	-1.91473500
C	2.82224400	0.15449500	0.66395400
C	-2.90240000	-0.68234200	-2.63704500
C	-4.14692900	-0.31828800	-3.14120900
C	-4.51922900	0.99251500	-2.83149500
C	3.46065100	1.16993700	1.38626400
C	4.70518000	0.80588300	1.89042800
C	5.07748100	-0.50491900	1.58071300
C	-5.73544600	1.68655800	-3.20056500
C	6.29369800	-1.19896200	1.94978300
C	-5.84217900	3.08700500	-3.08858500
C	-7.01194900	3.73730000	-3.44795300
C	-8.10146900	3.00648200	-3.92529700
C	-8.01243300	1.61824400	-4.04001000
C	-6.84456900	0.96229600	-3.68347700
C	6.40042900	-2.59940900	1.83780600
C	7.57020000	-3.24970300	2.19717400
C	8.65972200	-2.51888500	2.67451400
C	8.57068700	-1.13064600	2.78922300
C	7.40282200	-0.47469900	2.43269000
S	-3.27864400	1.76557300	-1.87987100
S	3.83689500	-1.27797700	0.62908900
H	1.12839900	2.26363900	0.52631900
H	-1.02488600	2.34632900	-0.56492300
H	-0.57014800	-1.77604300	-1.77710000
H	1.58313700	-1.85873300	-0.68585800
H	-2.46315100	-1.65590900	-2.79989000
H	-4.76122400	-0.97454500	-3.74011300
H	3.02140200	2.14350500	1.54911000
H	5.31947500	1.46214100	2.48933200
H	-4.99734900	3.66815200	-2.73811400
H	-7.07656800	4.81490300	-3.36264100
H	-9.01503300	3.51624000	-4.20581600
H	-8.85879400	1.04853300	-4.40317900
H	-6.79750900	-0.11627400	-3.75775700
H	5.55559800	-3.18055700	1.48733900
H	7.63481800	-4.32730700	2.11186500
H	9.57328500	-3.02864200	2.95503200
H	9.41704900	-0.56093600	3.15238900
H	7.35576300	0.60387100	2.50696700

5Sb compound

C	-0.98236200	0.03385600	-0.97698600
C	-1.33218800	-0.18579400	0.39738400
C	-0.31387600	-0.21374500	1.38672900
C	0.98235600	-0.03386100	0.97696500
C	1.33218300	0.18579000	-0.39740500
C	0.31387000	0.21374100	-1.38675000
C	3.45123100	0.25609700	0.61048900
C	2.71426700	0.34491600	-0.57304800
C	-3.45123600	-0.25610200	-0.61051000
C	-2.71427200	-0.34492100	0.57302700
C	4.88624200	0.36658400	0.75804400
C	-4.88624700	-0.36658900	-0.75806500
C	5.52846600	-0.03223900	1.94803700
C	6.90279400	0.07793300	2.07846900
C	7.66672800	0.59069200	1.02747400
C	7.04605600	0.99332100	-0.15657500
C	5.67204100	0.88261700	-0.29441300
C	-5.52847200	0.03223700	-1.94805700
C	-6.90280000	-0.07793500	-2.07848900
C	-7.66673300	-0.59069800	-1.02749500
C	-7.04606100	-0.99332900	0.15655300
C	-5.67204600	-0.88262600	0.29439100
H	-0.56992000	-0.37776400	2.42616400
H	0.56991400	0.37776000	-2.42618400
H	3.17549200	0.49713700	-1.53824100
H	-3.17549700	-0.49714200	1.53822000
H	4.94938100	-0.44833200	2.76389300
H	7.38396700	-0.23888000	2.99522200
H	8.74143400	0.67647300	1.13156500
H	7.63714200	1.39806500	-0.96853300
H	5.20307400	1.21842200	-1.20986600
H	-4.94938700	0.44833200	-2.76391200
H	-7.38397300	0.23887900	-2.99524200
H	-8.74143900	-0.67647900	-1.13158700
H	-7.63714700	-1.39807700	0.96850900
H	-5.20307900	-1.21843300	1.20984200
S	2.41642800	-0.02039800	1.99595600
S	-2.41643300	0.02039300	-1.99597700

5Sc compound

C	-5.65232700	-1.35626900	1.40069700
C	-6.03849500	0.01413200	1.43583700
C	-7.32381500	0.39745100	1.79587500
C	-8.23453800	-0.60341400	2.12504900
C	-7.87634100	-1.96624800	2.09779700
C	-6.60107900	-2.34924200	1.74071500
C	-4.30742300	-1.51786200	1.01004600
C	-3.64732000	-0.31834800	0.74390900
S	-4.71386800	1.06616900	0.98062600
C	-2.28688500	-0.15179200	0.32933900
C	-1.73734200	1.13457600	0.09241900
C	-0.43440600	1.29206100	-0.30471600
C	0.41681000	0.17091800	-0.49451600
C	-0.13273300	-1.11545100	-0.25759700
C	-1.43566900	-1.27293600	0.13953900
C	1.77724500	0.33747300	-0.90908600
S	2.84378800	-1.04704500	-1.14582400
C	4.16841800	0.00499400	-1.60102300
C	3.78225500	1.37539600	-1.56586300
C	2.43735300	1.53698900	-1.17520800
C	5.45373600	-0.37832500	-1.96106900
C	6.36446200	0.62254100	-2.29023000
C	6.00627000	1.98537500	-2.26295900
C	4.73101000	2.36837000	-1.90586900
H	-7.61511500	1.43964100	1.82187700
H	-9.24243300	-0.32589500	2.40872900
H	-8.61362100	-2.71393100	2.36063700
H	-6.31860800	-3.39480100	1.71753600
H	-3.83446600	-2.48601200	0.92585700
H	-2.35393400	2.01461300	0.22616300
H	-0.05820000	2.29150200	-0.47342200
H	0.48385900	-1.99548800	-0.39134000
H	-1.81187500	-2.27237600	0.30824500
H	1.96440000	2.50513900	-1.09100300
H	5.74503200	-1.42051600	-1.98708700
H	7.37235600	0.34502200	-2.57391700
H	6.74355300	2.73306000	-2.52578900
H	4.44854400	3.41393000	-1.88267500

5Sd compound

C	1.27331800	0.05987300	0.61792000
C	2.67563400	0.06058100	1.01026600
C	3.52437200	-0.23959900	-0.07928000
C	1.10990900	-0.24315500	-0.76517200
C	-0.14798700	-0.30496300	-1.38737200
C	-1.27331800	-0.05987300	-0.61791800
C	-1.10991000	0.24315600	0.76517400
C	0.14798600	0.30496400	1.38737400
C	3.25012200	0.30655200	2.25540900
C	4.63688100	0.25056000	2.39285700
C	5.45988500	-0.04849500	1.30105200
C	4.91213100	-0.29801400	0.04774800
C	-2.67563400	-0.06058100	-1.01026500
C	-3.52437300	0.23959900	0.07928000
C	-3.25012100	-0.30655200	-2.25540900
C	-4.63688000	-0.25056000	-2.39285800
C	-5.45988400	0.04849500	-1.30105400
C	-4.91213200	0.29801400	-0.04774900
H	-0.23088400	-0.53857400	-2.44165000
H	0.23088300	0.53857500	2.44165200
H	2.63080900	0.53972900	3.11305200
H	5.08379700	0.44165200	3.36038700
H	6.53388500	-0.08645800	1.43127500
H	5.54418800	-0.52977900	-0.80010500
H	-2.63080700	-0.53972900	-3.11305100
H	-5.08379500	-0.44165200	-3.36038800
H	-6.53388400	0.08645800	-1.43127700
H	-5.54418900	0.52977900	0.80010300
S	2.62261000	-0.51859900	-1.56118000
S	-2.62261200	0.51859900	1.56118100

5.3 Anionic ground state

4Oa compound

C	2.79806300	-0.45036600	-0.78196800
C	1.54802500	-1.04002100	-0.53430000
C	0.66895100	-0.00887000	-0.20347900
C	2.67241600	0.92224000	-0.60189300
C	-0.68941200	0.01926400	0.13801800
C	-2.69287700	-0.91184500	0.53643200
C	-2.81852400	0.46076000	0.71650700
C	-1.56848600	1.05041500	0.46883900
C	-3.59722900	-2.00585100	0.64336900
C	3.57676800	2.01624600	-0.70883000
C	-3.18145600	-3.34167900	0.39401000
C	-4.07205000	-4.39884200	0.50162800
C	-5.40959200	-4.18896600	0.85889100
C	-5.83442100	-2.87483100	1.10815000
C	-4.95783200	-1.80897400	1.00496700
C	3.16099500	3.35207300	-0.45947100
C	4.05158800	4.40923700	-0.56708900
C	5.38913100	4.19936100	-0.92435200
C	5.81396000	2.88522500	-1.17361100
C	4.93737100	1.81936800	-1.07042800
O	-1.37454800	-1.18301100	0.17842600
O	1.35408700	1.19340500	-0.24388700
H	3.70503200	-0.96284100	-1.06352800
H	1.28773200	-2.08485500	-0.58259000
H	-3.72549300	0.97323500	0.99806700
H	-1.30819300	2.09524900	0.51712800
H	-2.15080900	-3.52167600	0.11673700
H	-3.72027200	-5.40719900	0.30393400
H	-6.10033500	-5.02016400	0.94116500
H	-6.86697400	-2.68604100	1.38690900
H	-5.31419300	-0.80431400	1.20352800
H	2.13034800	3.53207000	-0.18219800
H	3.69981100	5.41759300	-0.36939500
H	6.07987300	5.03055900	-1.00662600
H	6.84651300	2.69643600	-1.45237000
H	5.29373200	0.81470900	-1.26898900

4Ob compound

C	0.97595900	0.96738200	1.08430600
C	-0.00427400	0.05514400	0.69450000
C	0.01287400	-0.06325100	-0.68653200
C	1.58577900	1.39526100	-0.11570700
C	-1.57717900	-1.40336800	0.12367500
C	-0.96735800	-0.97548900	-1.07633800
C	-2.62509500	-2.31118100	0.40476100
C	2.63369400	2.30307500	-0.39679300
C	-3.06126900	-2.57156300	1.73676000
C	-4.08873700	-3.46370200	1.99201500
C	-4.74048400	-4.14568500	0.95352100
C	-4.32266900	-3.90023700	-0.36401100
C	-3.29815800	-3.01268300	-0.63946200
C	3.06987000	2.56345800	-1.72879200
C	4.09733700	3.45559700	-1.98404600
C	4.74908400	4.13757900	-0.94555100
C	4.33126900	3.89213000	0.37198000
C	3.30675800	3.00457600	0.64743000
H	1.24323000	1.30147700	2.07282200
H	-1.23463000	-1.30958300	-2.06485400
H	-2.57242600	-2.05635800	2.55365600
H	-4.39269600	-3.63544900	3.02080200
H	-5.54399600	-4.84251700	1.16184000
H	-4.80999100	-4.41468600	-1.18746700
H	-3.00009800	-2.84618400	-1.66855200
H	2.58102700	2.04825300	-2.54568800
H	4.40129700	3.62734500	-3.01283300
H	5.55259600	4.83441200	-1.15386900
H	4.81859000	4.40657900	1.19543700
H	3.00869800	2.83807700	1.67652100
O	-0.96373300	-0.74960300	1.22371800
O	0.97233300	0.74149600	-1.21575000

4Oc compound

C	-5.21763000	-1.36236800	0.11569500
C	-6.33395700	-2.22206000	0.22418200
C	-7.60922700	-1.66491400	0.35125600
C	-7.81225000	-0.28156000	0.37412500
C	-6.71249700	0.59987000	0.26726300
C	-5.46149800	0.03850000	0.14254200
O	-4.28185500	0.72436500	0.02734200
C	-3.25874400	-0.23407800	-0.07557200
C	-3.81642000	-1.51811300	-0.02297100
C	-1.95934900	0.24869300	-0.20301300
C	-1.40167300	1.53272700	-0.25561400
C	-0.00046200	1.37698200	-0.39428100
C	0.24340500	-0.02388500	-0.42112700
O	-0.93623800	-0.70975100	-0.30592800
C	1.11586400	2.23667400	-0.50276800
C	2.39113400	1.67952800	-0.62984200
C	2.59415700	0.29617400	-0.65271100
C	1.49440400	-0.58525600	-0.54584900
H	-6.20283100	-3.29870300	0.20906300
H	-8.46745500	-2.32541100	0.43467600
H	-8.81434400	0.11986600	0.47391500
H	-6.83992300	1.67597800	0.28200000
H	-3.25342300	-2.43522400	-0.08044200
H	-1.96466900	2.44983800	-0.19814300
H	0.98473900	3.31331800	-0.48764900
H	3.24936300	2.34002600	-0.71326200
H	3.59625200	-0.10525200	-0.75250100
H	1.62183000	-1.66136400	-0.56058600

4Od compound

C	0.77561200	1.15002500	-1.08465600
C	-0.02600500	0.07395300	-0.68886300
C	0.01323800	-0.06393700	0.69022100
C	1.29868200	1.64692100	0.16317600
C	-1.31144900	-1.63690400	-0.16181700
C	-0.78837800	-1.14000800	1.08601400
C	-2.16181700	-2.70837900	-0.25662400
C	-2.54207600	-3.35817000	0.95266600
C	-2.05014200	-2.89798100	2.17841600
C	-1.18445200	-1.80775900	2.27921700
C	2.14905000	2.71839600	0.25798200
C	2.52930900	3.36818600	-0.95130700
C	2.03737600	2.90799700	-2.17705800
C	1.17168500	1.81777500	-2.27785900
H	-2.52527600	-3.04028600	-1.22206900
H	-3.21278200	-4.20872100	0.91753900
H	-2.35309000	-3.40841900	3.08878300
H	-0.81935800	-1.47352300	3.24272400
H	2.51250900	3.05030300	1.22342700
H	3.20001500	4.21873800	-0.91618100
H	2.34032400	3.41843600	-3.08742400
H	0.80659100	1.48354000	-3.24136500
O	-0.84409400	-0.89326800	-1.24572400
O	0.83132700	0.90328400	1.24708200

4Sa compound

C	2.52871300	1.05431500	-1.31914900
C	1.34013100	0.40065500	-0.98794500
C	0.32188800	1.25098500	-0.53117000
C	2.51324000	2.43759300	-1.14409500
C	-0.98476600	0.94021700	-0.11704100
C	-3.17611800	-0.24639100	0.49588400
C	-3.19159000	1.13688800	0.67093900
C	-2.00300800	1.79054700	0.33973500
C	-4.21398300	-1.20650900	0.73738700
C	3.55110400	3.39771200	-1.38559900
C	-4.02725500	-2.59355200	0.50423600
C	-5.03888500	-3.51328800	0.74158600
C	-6.28622700	-3.10547000	1.22176400
C	-6.49226100	-1.74016300	1.45891300
C	-5.48888900	-0.81432200	1.22513700
C	3.36437500	4.78475500	-1.15245100
C	4.37600500	5.70449200	-1.38980100
C	5.62334800	5.29667300	-1.86997700
C	5.82938200	3.93136600	-2.10712300
C	4.82601200	3.00552500	-1.87334600
S	-1.57855200	-0.73402100	-0.11689800
S	0.91567400	2.92522400	-0.53131400
H	3.40073900	0.52772700	-1.68576400
H	1.19937000	-0.66934300	-1.07064700
H	-4.06361600	1.66347600	1.03755400
H	-1.86224600	2.86054500	0.42243800
H	-3.07113400	-2.94292200	0.13181700
H	-4.85186400	-4.56537900	0.54911000
H	-7.07431500	-3.82638300	1.40609800
H	-7.45234100	-1.39635500	1.83205000
H	-5.68338000	0.23353500	1.41952700
H	2.40825300	5.13412500	-0.78003400
H	4.18898300	6.75658200	-1.19732800
H	6.41143500	6.01758700	-2.05431300
H	6.78946400	3.58755800	-2.48025800
H	5.02050400	1.95766800	-2.06773400

4Sb compound

C	1.24530800	0.97486600	0.87611000
C	0.19104000	0.08718700	0.67067000
C	-0.18775000	-0.09173800	-0.67530000
C	1.74240900	1.53476900	-0.31168600
C	-1.73912000	-1.53931800	0.30705700
C	-1.24201900	-0.97941500	-0.88074000
C	-2.80134300	-2.47621900	0.48762400
C	2.80463200	2.47166900	-0.49225300
C	-3.18716300	-2.95078600	1.77218600
C	-4.22056300	-3.86061000	1.93191100
C	-4.93048500	-4.35227700	0.83032100
C	-4.56732900	-3.89813900	-0.44583100
C	-3.53736000	-2.98980800	-0.61860200
C	3.54064600	2.98526200	0.61397400
C	4.57061400	3.89359400	0.44120300
C	4.93377400	4.34772800	-0.83495000
C	4.22385500	3.85605800	-1.93654000
C	3.19045500	2.94623400	-1.77681600
H	1.65119400	1.21845200	1.84792600
H	-1.64790500	-1.22300200	-1.85255500
H	-2.65981500	-2.59200700	2.64891600
H	-4.47913900	-4.19403300	2.93268900
H	-5.73790300	-5.06363800	0.95946400
H	-5.10072400	-4.26250700	-1.31906600
H	-3.28658600	-2.66287000	-1.62059900
H	3.28986900	2.65832600	1.61597000
H	5.10400700	4.25796400	1.31443800
H	5.74119100	5.05909000	-0.96409200
H	4.48243300	4.18947800	-2.93731900
H	2.66311000	2.58745100	-2.65354600
S	-0.82108100	-0.90158500	1.71412300
S	0.82437000	0.89703600	-1.71875200

4Sc compound

C	-5.41330700	-1.15128200	0.13565100
C	-6.43398300	-2.12994000	0.23435000
C	-7.76294100	-1.74782500	0.36621500
C	-8.13367000	-0.39610000	0.40554600
C	-7.14455000	0.59623700	0.31003700
C	-5.81917700	0.21963500	0.17853100
S	-4.42050800	1.29045000	0.04263600
C	-3.29635300	-0.10457400	-0.07144400
C	-4.01653800	-1.30696600	-0.00265000
C	-1.92174000	0.11918700	-0.20713600
C	-1.20155400	1.32158000	-0.27593500
C	0.19521400	1.16589600	-0.41423500
C	0.60108600	-0.20502100	-0.45711100
S	-0.79758400	-1.27583700	-0.32121200
C	1.21588900	2.14455400	-0.51294000
C	2.54484700	1.76244000	-0.64480700
C	2.91557800	0.41071500	-0.68413300
C	1.92645900	-0.58162200	-0.58861900
H	-6.16773000	-3.18172200	0.20586800
H	-8.53044000	-2.51260900	0.44029600
H	-9.17558600	-0.11518100	0.50888100
H	-7.41702000	1.64617300	0.33905700
H	-3.52714700	-2.27112600	-0.05300100
H	-1.69094700	2.28573900	-0.22558800
H	0.94963500	3.19633600	-0.48446200
H	3.31234500	2.52722500	-0.71889100
H	3.95749300	0.12979700	-0.78746900
H	2.19892900	-1.63155800	-0.61763600

4Sd compound

C	0.87381900	1.25049100	-0.99896400
C	0.05257200	0.16032900	-0.68314900
C	-0.05259000	-0.16031900	0.68314900
C	1.45003300	1.82293200	0.18930000
C	-1.45005000	-1.82292300	-0.18930000
C	-0.87383700	-1.25048200	0.99896500
C	-2.29779100	-2.90972500	-0.14599900
C	-2.61784000	-3.48839600	1.10383600
C	-2.06773100	-2.94671400	2.27406200
C	-1.21264500	-1.85244300	2.24441800
C	2.29777400	2.90973300	0.14599900
C	2.61782400	3.48840400	-1.10383600
C	2.06771400	2.94672200	-2.27406200
C	1.21262800	1.85245100	-2.24441800
H	-2.71523600	-3.31701600	-1.06115800
H	-3.28286100	-4.34285400	1.15176600
H	-2.31629300	-3.39441500	3.23233500
H	-0.79921700	-1.45070500	3.16309000
H	2.71522000	3.31702400	1.06115800
H	3.28284500	4.34286100	-1.15176600
H	2.31627700	3.39442300	-3.23233600
H	0.79920100	1.45071300	-3.16309000
S	-0.92417200	-0.95182100	-1.65798600
S	0.92415400	0.95183000	1.65798600

5Oa compound

C	0.54746600	1.20680000	0.45483800
C	-0.73580500	1.18155300	-0.03813400
C	-1.33184400	-0.02718100	-0.49549000
C	-0.53634000	-1.20345300	-0.41727200
C	0.74693100	-1.17820500	0.07569900
C	1.34297000	0.03052900	0.53305500
C	-2.65762700	-0.06437700	-1.00706100
C	2.66875300	0.06772400	1.04462600
C	-3.46401800	-1.08293800	-1.50828700
C	-4.69749700	-0.50532100	-1.86763100
C	-4.62863800	0.84675900	-1.58354800
C	3.47514400	1.08628600	1.54585300
C	4.70862300	0.50866800	1.90519600
C	4.63976500	-0.84341100	1.62111300
C	-5.54526800	1.93689600	-1.72465200
C	5.55639400	-1.93354800	1.76221700
C	-5.19011700	3.25218200	-1.33936000
C	-6.08620500	4.30266400	-1.48036000
C	-7.36460800	4.09464900	-2.00616300
C	-7.72877500	2.79791000	-2.39128900
C	-6.84363300	1.74085400	-2.25568000
C	5.20124300	-3.24883400	1.37692500
C	6.09733100	-4.29931600	1.51792500
C	7.37573500	-4.09130100	2.04372800
C	7.73990100	-2.79456200	2.42885400
C	6.85475900	-1.73750600	2.29324500
O	-3.37672500	1.11482300	-1.05586700
O	3.38785200	-1.11147500	1.09343200
H	0.96221700	2.15048200	0.79265000
H	-1.31316700	2.09665400	-0.08317100
H	-0.95109100	-2.14713400	-0.75508500
H	1.32429300	-2.09330600	0.12073600
H	-3.18415600	-2.11994100	-1.59958900
H	-5.54886200	-1.01684900	-2.28927700
H	3.19528200	2.12328900	1.63715400
H	5.55998800	1.02019600	2.32684200
H	-4.20329800	3.42678600	-0.93087900
H	-5.78436100	5.29992900	-1.17586500
H	-8.06015200	4.91885400	-2.11394000
H	-8.71667700	2.61403600	-2.80195400
H	-7.14899500	0.74641300	-2.56085600
H	4.21442400	-3.42343800	0.96844400
H	5.79548800	-5.29658100	1.21343100
H	8.07127900	-4.91550600	2.15150500
H	8.72780300	-2.61068800	2.83952000
H	7.16012100	-0.74306500	2.59842200

5Ob compound

C	0.48227400	-1.29990200	0.18746700
C	-0.28321300	-0.13390400	-0.07100900
C	0.38404400	1.11654100	-0.22779500
C	1.74763700	1.30087000	-0.14848300
C	2.51312300	0.13487300	0.10999400
C	1.84586700	-1.11557300	0.26677900
C	3.89237200	-0.14501900	0.26882300
C	4.03280800	-1.50457800	0.50937300
O	2.76721600	-2.10085300	0.50745200
C	-1.66246100	0.14598800	-0.22983900
C	-1.80289700	1.50554600	-0.47038900
O	-0.53730500	2.10182200	-0.46846700
C	5.15583900	-2.34928800	0.74298300
C	-2.92592800	2.35025700	-0.70399800
C	5.00647700	-3.74364000	0.96665600
C	6.10882700	-4.55284200	1.19278000
C	7.40603500	-4.02391000	1.20839900
C	7.56872700	-2.64837600	0.98898800
C	6.47777400	-1.82724200	0.76178100
C	-2.77656600	3.74460800	-0.92767200
C	-3.87891600	4.55381000	-1.15379600
C	-5.17612400	4.02487800	-1.16941500
C	-5.33881700	2.64934400	-0.95000400
C	-4.24786300	1.82821000	-0.72279700
H	0.03026500	-2.27524800	0.31528000
H	2.19964500	2.27621600	-0.27629600
H	4.70294500	0.56495300	0.21491700
H	-2.47303400	-0.56398500	-0.17593300
H	4.01073300	-4.16771500	0.95783200
H	5.95889700	-5.61523900	1.36032000
H	8.26399500	-4.66199100	1.38579000
H	8.56469700	-2.21571700	0.99651000
H	6.63241100	-0.76735400	0.59512900
H	-1.78082300	4.16868400	-0.91884800
H	-3.72898700	5.61620800	-1.32133600
H	-6.03408400	4.66295900	-1.34680600
H	-6.33478600	2.21668500	-0.95752600
H	-4.40250000	0.76832200	-0.55614500

5Oc compound

C	-5.53349200	-1.65316100	1.38191500
C	-5.66876400	-0.24356800	1.34059300
C	-6.83469400	0.42580000	1.64909300
C	-7.94304600	-0.35398100	2.02443800
C	-7.84424500	-1.74962600	2.07587600
C	-6.65671200	-2.41198400	1.76048900
C	-4.18998400	-1.92619100	0.99761900
C	-3.56907200	-0.70832000	0.74231800
O	-4.48909900	0.32773800	0.95625300
C	-2.26247900	-0.34431400	0.33253200
C	-1.87767000	1.01503700	0.13991200
C	-0.60778700	1.35288400	-0.25711900
C	0.39240400	0.36344100	-0.49771000
C	0.00759500	-0.99591100	-0.30509100
C	-1.26228800	-1.33375800	0.09193900
C	1.69899800	0.72744600	-0.90749400
O	2.61902200	-0.30861200	-1.12143600
C	3.79868900	0.26269400	-1.50577200
C	3.66342000	1.67228800	-1.54708300
C	2.31991200	1.94531800	-1.16278700
C	4.96461800	-0.40667400	-1.81427500
C	6.07297100	0.37310600	-2.18961400
C	5.97417400	1.76875300	-2.24104200
C	4.78664200	2.43111100	-1.92565100
H	-6.88598500	1.50699200	1.60175800
H	-8.87913500	0.13170800	2.27513700
H	-8.71338900	-2.33027200	2.36845400
H	-6.60114600	-3.49413900	1.80666500
H	-3.72288500	-2.89391700	0.91462800
H	-2.61120600	1.79267000	0.31343200
H	-0.35903700	2.40003700	-0.39123600
H	0.74113100	-1.77354300	-0.47861200
H	-1.51103800	-2.38091000	0.22605600
H	1.85281600	2.91304500	-1.07978800
H	5.01590600	-1.48786700	-1.76694800
H	7.00905900	-0.11258200	-2.44031600
H	6.84331900	2.34939800	-2.53361500
H	4.73107800	3.51326600	-1.97182000

5Od compound

C	0.76164200	1.32190300	0.31725000
C	1.62015200	0.19920300	0.11844900
C	1.04837800	-1.07139300	-0.15966300
C	-0.29930900	-1.33366300	-0.25939600
C	-1.15781900	-0.21096300	-0.06059600
C	-0.58604400	1.05963300	0.21751600
C	-2.56895100	-0.01806600	-0.06988000
C	-2.78610700	1.35824900	0.20263800
O	-1.58540200	2.01315000	0.37713000
C	3.03128400	0.00630600	0.12773400
C	3.24844100	-1.37000900	-0.14478500
O	2.04773500	-2.02491000	-0.31927700
C	-3.70147500	-0.83704500	-0.27547800
C	-4.97125500	-0.26088700	-0.20201300
C	-5.15001200	1.10057900	0.06881100
C	-4.03058600	1.93943600	0.27802900
C	4.16380900	0.82528500	0.33333200
C	5.43358900	0.24912700	0.25986700
C	5.61234600	-1.11233900	-0.01095700
C	4.49292000	-1.95119600	-0.22017500
H	1.13889400	2.31293800	0.53185400
H	-0.67656100	-2.32469800	-0.47400000
H	-3.58588600	-1.89417100	-0.48654800
H	-5.84511400	-0.88615300	-0.35931000
H	-6.14930700	1.51770900	0.11926700
H	-4.13983300	2.99653000	0.48933900
H	4.04821900	1.88241100	0.54440100
H	6.30744800	0.87439300	0.41716400
H	6.61164000	-1.52946900	-0.06141400
H	4.60216600	-3.00829000	-0.43148500

5Sa compound

C	0.80683200	1.40274700	-0.07292500
C	-0.43319700	1.43280500	-0.66771700
C	-1.02074100	0.27595900	-1.24870000
C	-0.24857900	-0.91515000	-1.17785900
C	0.99144900	-0.94520800	-0.58306600
C	1.57899300	0.21163700	-0.00208300
C	-2.30849100	0.29640800	-1.86920500
C	2.86674300	0.19118900	0.61842200
C	-3.01710700	-0.74260300	-2.47745300
C	-4.26680300	-0.37062100	-2.99035200
C	-4.59721100	0.96674400	-2.81123400
C	3.57535900	1.23020000	1.22666900
C	4.82505500	0.85821700	1.73956800
C	5.15546300	-0.47914700	1.56045100
C	-5.78788500	1.67436900	-3.21030400
C	6.34613600	-1.18677300	1.95952300
C	-5.96706100	3.05220400	-2.94164500
C	-7.11831900	3.72350200	-3.33099400
C	-8.14405100	3.05748600	-4.00465000
C	-7.98649200	1.69461400	-4.28002500
C	-6.83997600	1.01753900	-3.89466900
C	6.52531100	-2.56460800	1.69086600
C	7.67656800	-3.23590600	2.08021600
C	8.70230100	-2.56989100	2.75387000
C	8.54474300	-1.20701800	3.02924300
C	7.39822900	-0.52994200	2.64388600
S	-3.27308800	1.77850900	-1.96167200
S	3.83134000	-1.29091200	0.71089000
H	1.20091200	2.31815400	0.35267000
H	-0.97674400	2.37120400	-0.69187900
H	-0.64266000	-1.83055700	-1.60345300
H	1.53499700	-1.88360700	-0.55890400
H	-2.62908000	-1.74979400	-2.54425900
H	-4.92514200	-1.07141600	-3.48766900
H	3.18733200	2.23739100	1.29347500
H	5.48339400	1.55901200	2.23688600
H	-5.18829400	3.59619000	-2.41988400
H	-7.21635200	4.78064600	-3.10556500
H	-9.04182100	3.58364500	-4.30760500
H	-8.76997400	1.15500700	-4.80279800
H	-6.74890300	-0.03721700	-4.12362500
H	5.74654300	-3.10859500	1.16910600
H	7.77460000	-4.29305100	1.85478900
H	9.60007100	-3.09605000	3.05682600
H	9.32822600	-0.66741100	3.55201500
H	7.30715600	0.52481400	2.87283900

5Sb compound

C	-1.00244900	0.15144000	-0.93689800
C	-1.33964700	-0.26790900	0.39234000
C	-0.28981700	-0.41576800	1.33603900
C	1.00244300	-0.15144000	0.93687900
C	1.33964100	0.26790900	-0.39235900
C	0.28981200	0.41576800	-1.33605800
C	3.50204200	0.24346500	0.57148600
C	2.72579800	0.47598800	-0.55682700
C	-3.50204700	-0.24346800	-0.57150700
C	-2.72580300	-0.47599000	0.55680800
C	4.92193500	0.36027800	0.73885000
C	-4.92194000	-0.36028400	-0.73887100
C	5.56318100	0.07920800	1.97308300
C	6.93719300	0.19599300	2.12142000
C	7.74595800	0.59753700	1.05324400
C	7.13316400	0.88015200	-0.17468700
C	5.76208700	0.76664900	-0.33304200
C	-5.56318600	-0.07920800	-1.97310300
C	-6.93719800	-0.19599600	-2.12144100
C	-7.74596300	-0.59754600	-1.05326600
C	-7.13316800	-0.88016700	0.17466200
C	-5.76209200	-0.76666200	0.33301800
H	-0.51203400	-0.73142100	2.34941200
H	0.51202800	0.73142100	-2.34943100
H	3.15370700	0.79476200	-1.49872900
H	-3.15371300	-0.79476400	1.49870900
H	4.96520100	-0.23469200	2.82104000
H	7.38597700	-0.02924400	3.08402600
H	8.81944100	0.68796600	1.17189800
H	7.73858400	1.19393900	-1.01971200
H	5.32176100	0.99327800	-1.29634800
H	-4.96520700	0.23469700	-2.82105800
H	-7.38598200	0.02924500	-3.08404600
H	-8.81944600	-0.68797800	-1.17192100
H	-7.73858800	-1.19396000	1.01968600
H	-5.32176500	-0.99329600	1.29632300
S	2.45711800	-0.26666500	1.93089300
S	-2.45712300	0.26666400	-1.93091300

5Sc compound

C	-5.69254800	-1.38192900	1.41402200
C	-6.08437900	-0.01259900	1.45119000
C	-7.36602100	0.37989400	1.80979500
C	-8.30677700	-0.59978600	2.14648700
C	-7.94553500	-1.95459200	2.11752000
C	-6.66305300	-2.34891200	1.75880100
C	-4.33920800	-1.55226500	1.02137500
C	-3.65513500	-0.37195600	0.74944200
S	-4.74335300	1.03000000	0.99184400
C	-2.30483800	-0.17485900	0.33604500
C	-1.75263400	1.11622200	0.09746000
C	-0.45005100	1.29425000	-0.30077700
C	0.43476400	0.19398600	-0.50122000
C	-0.11744000	-1.09709500	-0.26263500
C	-1.42002300	-1.27512400	0.13560200
C	1.78506100	0.39108200	-0.91461700
S	2.87327800	-1.01087400	-1.15701900
C	4.21430500	0.03172500	-1.61636500
C	3.82247400	1.40105500	-1.57919700
C	2.46913400	1.57139200	-1.18655000
C	5.49594700	-0.36076800	-1.97496900
C	6.43670400	0.61891200	-2.31166000
C	6.07546200	1.97371800	-2.28269200
C	4.79298000	2.36803800	-1.92397300
H	-7.63518100	1.43044600	1.82898600
H	-9.31217800	-0.30896900	2.42875300
H	-8.68130700	-2.70806600	2.38010300
H	-6.39863600	-3.40117200	1.74114000
H	-3.87359900	-2.52483700	0.93940300
H	-2.37804900	1.99242900	0.23353600
H	-0.08931500	2.30273100	-0.46591500
H	0.50797500	-1.97330300	-0.39871100
H	-1.78075900	-2.28360500	0.30074000
H	2.00352600	2.54396300	-1.10457700
H	5.76510700	-1.41132000	-1.99416100
H	7.44210500	0.32809500	-2.59392500
H	6.81123400	2.72719200	-2.54527300
H	4.52856400	3.42029800	-1.90631100

5Sd compound

C	1.29497200	0.05167700	0.58777600
C	2.66715800	0.05208500	0.97042400
C	3.55080900	-0.24769500	-0.10765100
C	1.09851400	-0.24848600	-0.79187400
C	-0.14288400	-0.30589900	-1.39013000
C	-1.29497200	-0.05167700	-0.58777500
C	-1.09851400	0.24848600	0.79187400
C	0.14288400	0.30589900	1.39013000
C	3.24911300	0.30268800	2.23806200
C	4.62966300	0.25148800	2.39491400
C	5.47620800	-0.04544000	1.31907900
C	4.92393200	-0.29847700	0.04902000
C	-2.66715800	-0.05208500	-0.97042400
C	-3.55080900	0.24769500	0.10765100
C	-3.24911300	-0.30268800	-2.23806200
C	-4.62966300	-0.25148800	-2.39491400
C	-5.47620800	0.04544000	-1.31907900
C	-4.92393200	0.29847700	-0.04902000
H	-0.24885400	-0.53775900	-2.44307000
H	0.24885400	0.53775900	2.44307000
H	2.61249900	0.53445900	3.08472700
H	5.05998100	0.44597200	3.37277700
H	6.55052900	-0.08116300	1.45926700
H	5.56657100	-0.52976000	-0.79376200
H	-2.61249900	-0.53445900	-3.08472700
H	-5.05998100	-0.44597200	-3.37277700
H	-6.55052900	0.08116300	-1.45926800
H	-5.56657100	0.52976000	0.79376200
S	2.65347500	-0.53174500	-1.61071900
S	-2.65347500	0.53174500	1.61071900

4. S_1 ground state

4Oa compound

C	2.77569500	-0.46897100	-0.77944000
C	1.53381400	-1.05293100	-0.53320700
C	0.66712200	-0.01062400	-0.20378600
C	2.63313500	0.90523400	-0.59480000
C	-0.68775300	0.02108700	0.13761700
C	-2.65372000	-0.89478700	0.52881700
C	-2.79628200	0.47941900	0.71344400
C	-1.55447600	1.06341000	0.46690700
C	-3.55769700	-1.98907200	0.63568400
C	3.53720700	1.99947800	-0.70126900
C	-3.12898100	-3.31479200	0.38455500
C	-4.01739000	-4.36844800	0.49188000
C	-5.34851500	-4.14558900	0.84852000
C	-5.78360300	-2.83973300	1.09910800
C	-4.90990500	-1.77658200	0.99646300
C	3.10851700	3.32518200	-0.45000600
C	3.99702800	4.37879500	-0.55689800
C	5.32824500	4.15590400	-0.91317500
C	5.76331400	2.85006200	-1.16386900
C	4.88949800	1.78696000	-1.06171800
O	-1.35974500	-1.16824400	0.17626600
O	1.33912600	1.17870200	-0.24238300
H	3.68603400	-0.97484500	-1.06122000
H	1.26485300	-2.09694900	-0.57935300
H	-3.70656400	0.98527000	0.99545100
H	-1.28552500	2.10743300	0.51300600
H	-2.09666000	-3.49418400	0.10724800
H	-3.67279000	-5.37908100	0.29599300
H	-6.04015900	-4.97723100	0.93084300
H	-6.81698000	-2.65789800	1.37693500
H	-5.26364100	-0.77004900	1.19422200
H	2.07613000	3.50459600	-0.17296000
H	3.65244500	5.38941600	-0.36092100
H	6.01996800	4.98751300	-0.99516400
H	6.79674800	2.66820800	-1.44146800
H	5.24320400	0.78044400	-1.25962200

4Ob compound

C	0.96791600	0.96063100	1.08741500
C	-0.00749100	0.05238300	0.69549300
C	0.01606500	-0.06046200	-0.68753100
C	1.55890900	1.37085100	-0.12212700
C	-1.55033000	-1.37893600	0.13009100
C	-0.95935700	-0.96869500	-1.07945400
C	-2.60164500	-2.29007800	0.40773000
C	2.61023700	2.28198100	-0.39976300
C	-3.02421300	-2.53853100	1.73845900
C	-4.04901100	-3.42853600	1.99011400
C	-4.68724900	-4.09929900	0.94127300
C	-4.27957100	-3.86280500	-0.37560000
C	-3.25738600	-2.97714700	-0.64824500
C	3.03288800	2.53034400	-1.73048200
C	4.05771700	3.42031500	-1.98213200
C	4.69587700	4.09116400	-0.93329800
C	4.28810900	3.85476600	0.38356400
C	3.26591000	2.96912200	0.65620600
H	1.24236200	1.30084200	2.07212800
H	-1.23381400	-1.30889300	-2.06416800
H	-2.53335400	-2.02168700	2.55499800
H	-4.36054700	-3.60752200	3.01439400
H	-5.49182100	-4.79727300	1.14702400
H	-4.77060900	-4.37995700	-1.19399700
H	-2.95425200	-2.80594400	-1.67588200
H	2.54207900	2.01344600	-2.54701800
H	4.36932300	3.59922500	-3.00640500
H	5.50046200	4.78912300	-1.13904600
H	4.77908900	4.37198100	1.20195700
H	2.96271400	2.79798700	1.68383500
O	-0.95716200	-0.74434900	1.21847700
O	0.96575200	0.73625300	-1.21051300

4Oc compound

C	-5.19414200	-1.35755300	0.11334500
C	-6.30907400	-2.22708700	0.22162700
C	-7.56494600	-1.66432700	0.34674600
C	-7.75473200	-0.27090600	0.36834600
C	-6.67365400	0.61441700	0.26342600
C	-5.42671600	0.04382000	0.13914900
O	-4.25416800	0.72329700	0.02478600
C	-3.26443900	-0.22510000	-0.07481400
C	-3.80573200	-1.51673600	-0.02399100
C	-1.95360500	0.23971400	-0.20327700
C	-1.41232700	1.53135000	-0.25425600
C	-0.02394100	1.37216700	-0.39184000
C	0.20863800	-0.02920600	-0.41758600
O	-0.96388600	-0.70868300	-0.30298000
C	1.09096400	2.24170100	-0.50039400
C	2.34681900	1.67894200	-0.62568200
C	2.53661700	0.28552000	-0.64716100
C	1.45556400	-0.59980300	-0.54198200
H	-6.17436300	-3.30284900	0.20614100
H	-8.43296200	-2.31024900	0.43111900
H	-8.75862100	0.12796000	0.46827100
H	-6.80497000	1.68985200	0.27858700
H	-3.23191800	-2.42903900	-0.08248300
H	-1.98614300	2.44365300	-0.19578500
H	0.95624500	3.31746400	-0.48498500
H	3.21481400	2.32486400	-0.71026800
H	3.54049400	-0.11334600	-0.74720300
H	1.58688800	-1.67523800	-0.55705600

4Od compound

C	0.77349000	1.14756900	-1.08622300
C	-0.03173800	0.06821300	-0.70056000
C	0.01902400	-0.05823800	0.70191200
C	1.27922800	1.62324900	0.15511800
C	-1.29195700	-1.61326100	-0.15376400
C	-0.78623900	-1.13756600	1.08757900
C	-2.14385000	-2.68375200	-0.26997500
C	-2.51235400	-3.31863500	0.94060800
C	-2.03365900	-2.87647400	2.17541200
C	-1.17139500	-1.79214700	2.28704200
C	2.13112400	2.69373700	0.27132900
C	2.49959300	3.32864700	-0.93925000
C	2.02084700	2.88652600	-2.17404900
C	1.15857400	1.80220600	-2.28567900
H	-2.50845900	-3.01743100	-1.23304300
H	-3.18377100	-4.16963500	0.90263200
H	-2.34662100	-3.39801500	3.07401000
H	-0.80211800	-1.45204300	3.24664000
H	2.49575400	3.02739900	1.23439400
H	3.17101700	4.17964200	-0.90127600
H	2.33377100	3.40809800	-3.07264300
H	0.78925500	1.46213500	-3.24527100
O	-0.82112500	-0.86516100	-1.23751400
O	0.80840900	0.87513800	1.23886600

4Sa compound

C	2.50701200	1.02256300	-1.31608300
C	1.32443100	0.37585200	-0.98814100
C	0.32049000	1.24784000	-0.53567900
C	2.47181900	2.41003100	-1.13411100
C	-0.98632000	0.94441800	-0.12101500
C	-3.13558500	-0.21850800	0.48333900
C	-3.17129700	1.16913700	0.66385300
C	-1.98987100	1.81626100	0.33258500
C	-4.17099600	-1.18012500	0.72578800
C	3.50826100	3.37128000	-1.37359700
C	-3.96747500	-2.55964600	0.49127800
C	-4.97242200	-3.47947600	0.72814100
C	-6.21464600	-3.06449700	1.20581800
C	-6.43548900	-1.70642600	1.44370800
C	-5.43836500	-0.77933700	1.21038600
C	3.30711500	4.74996900	-1.13223900
C	4.31295300	5.66947800	-1.36654500
C	5.55379200	5.25497700	-1.84822100
C	5.77230300	3.89772400	-2.09283000
C	4.77421600	2.97097900	-1.86227500
S	-1.56879800	-0.70857100	-0.11964400
S	0.90386400	2.90051300	-0.53450500
H	3.38381900	0.50395100	-1.68104300
H	1.17235800	-0.69405500	-1.06654300
H	-4.04741000	1.68749500	1.03083400
H	-1.83819600	2.88630700	0.40985800
H	-3.00766200	-2.90573300	0.11941300
H	-4.78820400	-4.53229400	0.53927500
H	-7.00108900	-3.78841300	1.39072200
H	-7.39870800	-1.37163400	1.81553400
H	-5.63540700	0.26929200	1.40287200
H	2.34859400	5.09560700	-0.75664500
H	4.13058600	6.72164800	-1.17234500
H	6.34095500	5.97863500	-2.03105900
H	6.73435700	3.56333600	-2.46802300
H	4.96920500	1.92306900	-2.06067300

4Sb compound

C	1.23247600	0.96080900	0.89018700
C	0.18321300	0.07887000	0.67758800
C	-0.18015500	-0.08315200	-0.68218300
C	1.71530500	1.51114400	-0.30809700
C	-1.71219000	-1.51549300	0.30349400
C	-1.22939700	-0.96511600	-0.89478600
C	-2.77388000	-2.45185300	0.48075500
C	2.77708900	2.44739500	-0.48537200
C	-3.14482600	-2.91546000	1.76895800
C	-4.17421400	-3.82218500	1.92969300
C	-4.87553800	-4.30467300	0.82305300
C	-4.52591100	-3.86053400	-0.45553800
C	-3.49971100	-2.95487800	-0.63108500
C	3.50305600	2.95026800	0.62644900
C	4.52937500	3.85578500	0.45088400
C	4.87901900	4.29990100	-0.82771100
C	4.17758900	3.81753300	-1.93433600
C	3.14805800	2.91097300	-1.77357900
H	1.64358500	1.20757900	1.85900000
H	-1.64049600	-1.21189800	-1.86359900
H	-2.61311800	-2.55366100	2.64407800
H	-4.43724700	-4.16021600	2.92696300
H	-5.68334500	-5.01678500	0.95375800
H	-5.06523400	-4.22986300	-1.32211000
H	-3.24828900	-2.62634500	-1.63335300
H	3.25166300	2.62170400	1.62871500
H	5.06880200	4.22499600	1.31744100
H	5.68693200	5.01189000	-0.95843200
H	4.44063500	4.15554500	-2.93160800
H	2.61626000	2.54927500	-2.64868600
S	-0.81898800	-0.90091100	1.70597400
S	0.82210000	0.89656600	-1.71057700

4Sc compound

C	-5.38201300	-1.15065500	0.13491700
C	-6.40076700	-2.13217900	0.23872000
C	-7.70157700	-1.74339100	0.36840300
C	-8.05406200	-0.38264900	0.40129700
C	-7.08462000	0.60731900	0.30256200
C	-5.76819200	0.22718000	0.17121900
S	-4.39066000	1.28747000	0.03119300
C	-3.29858200	-0.09542100	-0.07610000
C	-4.00048300	-1.31363600	-0.00415800
C	-1.92142900	0.10990900	-0.21193200
C	-1.22000800	1.32816500	-0.28804500
C	0.16245000	1.16530800	-0.41861600
C	0.54987000	-0.21265600	-0.44657600
S	-0.82806300	-1.27283500	-0.30719900
C	1.18156900	2.14728400	-0.52145100
C	2.48500400	1.75831400	-0.64361000
C	2.83856400	0.39712600	-0.66927100
C	1.86848900	-0.59318100	-0.57016200
H	-6.13499800	-3.18366300	0.21417100
H	-8.48062700	-2.49390900	0.44782700
H	-9.09604500	-0.10022700	0.50490600
H	-7.36164900	1.65549800	0.32839900
H	-3.50087500	-2.27393100	-0.05630900
H	-1.72098500	2.28837200	-0.24881200
H	0.91497000	3.19872700	-0.50173100
H	3.26414200	2.50892800	-0.72226400
H	3.88112400	0.11472600	-0.76753700
H	2.14615300	-1.64139200	-0.59003900

4Sd compound

C	0.87606500	1.25548900	-1.01470100
C	0.04754500	0.15473900	-0.68946100
C	-0.04755100	-0.15473900	0.68945900
C	1.43974600	1.81319800	0.16455400
C	-1.43975500	-1.81319600	-0.16455500
C	-0.87607500	-1.25548600	1.01470000
C	-2.28793700	-2.89659100	-0.15002600
C	-2.60667600	-3.47399300	1.10284900
C	-2.06803700	-2.94635000	2.26844800
C	-1.20748600	-1.84677500	2.25093800
C	2.28792500	2.89659600	0.15002600
C	2.60665400	3.47400700	-1.10284800
C	2.06801200	2.94636500	-2.26844700
C	1.20747100	1.84678300	-2.25093900
H	-2.70239900	-3.29983600	-1.06710300
H	-3.27221100	-4.32815000	1.14405100
H	-2.32036200	-3.39826900	3.22242500
H	-0.79911500	-1.45222800	3.17489000
H	2.70238500	3.29984100	1.06710300
H	3.27217900	4.32817000	-1.14404900
H	2.32033000	3.39829000	-3.22242300
H	0.79909800	1.45223700	-3.17489100
S	-0.90347300	-0.93203200	-1.61073200
S	0.90346700	0.93203200	1.61073000

5Oa compound

C	0.54401900	1.21289200	0.45410900
C	-0.73412400	1.18590700	-0.03743800
C	-1.31684800	-0.02833300	-0.49018100
C	-0.53292300	-1.20959700	-0.41653000
C	0.74521800	-1.18261200	0.07502700
C	1.32794200	0.03162900	0.52776700
C	-2.63756800	-0.06456400	-0.99976900
C	2.64865800	0.06787100	1.03736500
C	-3.43871400	-1.09057700	-1.50017500
C	-4.66029100	-0.51636100	-1.85569700
C	-4.57693900	0.83849700	-1.56570000
C	3.44978300	1.09389500	1.53778500
C	4.67136300	0.51969600	1.89332100
C	4.58802900	-0.83516400	1.60333300
C	-5.49261900	1.92588500	-1.70695200
C	5.50374000	-1.92253200	1.74455300
C	-5.13115500	3.23446400	-1.32037100
C	-6.02658100	4.27994500	-1.46178200
C	-7.29891600	4.06018000	-1.98745300
C	-7.66785700	2.76924300	-2.37353200
C	-6.78393900	1.71658300	-2.23779400
C	5.14233500	-3.23109900	1.35787800
C	6.03780200	-4.27655200	1.49922700
C	7.31012300	-4.05677000	2.02492600
C	7.67900400	-2.76584600	2.41110200
C	6.79504300	-1.71321400	2.27543000
O	-3.34436900	1.10408100	-1.04604300
O	3.35547000	-1.10076600	1.08365900
H	0.96261700	2.15475700	0.79251300
H	-1.31643600	2.09847400	-0.08549800
H	-0.95151700	-2.15145900	-0.75494500
H	1.32753800	-2.09517600	0.12306600
H	-3.15673400	-2.12831000	-1.59068100
H	-5.51551100	-1.02167500	-2.27754600
H	3.16779000	2.13162500	1.62828100
H	5.52657600	1.02502400	2.31516800
H	-4.14346900	3.41162600	-0.91105400
H	-5.73181000	5.27991200	-1.15928600
H	-7.99668200	4.88364100	-2.09597600
H	-8.65630000	2.58847500	-2.78376400
H	-7.08639400	0.72014900	-2.54239000
H	4.15466200	-3.40827400	0.94853500
H	5.74307900	-5.27651000	1.19665400
H	8.00792400	-4.88020800	2.13339600
H	8.66743300	-2.58506500	2.82136300
H	7.09745300	-0.71678700	2.58009600

5Ob compound

C	0.48247700	-1.30584400	0.18887500
C	-0.27095400	-0.13185900	-0.07027100
C	0.39392600	1.11865400	-0.22745800
C	1.74741200	1.30686800	-0.14958300
C	2.50084200	0.13288500	0.10956700
C	1.83596200	-1.11762900	0.26675100
C	3.86853700	-0.14416500	0.26708800
C	3.98763300	-1.51404700	0.50789200
O	2.75267900	-2.09682600	0.50623800
C	-1.63864300	0.14517800	-0.22785800
C	-1.75773700	1.51505500	-0.46869200
O	-0.52278800	2.09784300	-0.46698600
C	5.11632000	-2.34931100	0.74017900
C	-2.88641400	2.35029100	-0.70113100
C	4.96640800	-3.73875300	0.96273100
C	6.07279100	-4.53408600	1.18640300
C	7.35787900	-3.98246600	1.19705000
C	7.51889500	-2.61173500	0.97863000
C	6.42347800	-1.80207200	0.75340900
C	-2.73649700	3.73971500	-0.92379100
C	-3.84286300	4.53500400	-1.14770600
C	-5.12794000	3.98336000	-1.15847300
C	-5.28896600	2.61265800	-0.93988200
C	-4.19356600	1.80303900	-0.71442000
H	0.02294200	-2.27790700	0.31569400
H	2.20695000	2.27892500	-0.27644600
H	4.68726800	0.55663700	0.21515600
H	-2.45736900	-0.55563400	-0.17598100
H	3.97249700	-4.17107000	0.95547400
H	5.94036400	-5.59807500	1.35537600
H	8.22269000	-4.61307700	1.37337600
H	8.51316400	-2.17628500	0.98541600
H	6.56619300	-0.73979300	0.58552600
H	-1.74259300	4.17204600	-0.91646300
H	-3.71042900	5.59897300	-1.31680400
H	-5.99273500	4.61393300	-1.33501500
H	-6.28322700	2.17719200	-0.94674900
H	-4.33628700	0.74077800	-0.54642600

5Oc compound

C	-5.49275700	-1.63847900	1.36915600
C	-5.62654200	-0.23133700	1.32741900
C	-6.79055700	0.43724500	1.63513900
C	-7.88222300	-0.35195700	2.00583600
C	-7.78705400	-1.75202600	2.05869600
C	-6.61105000	-2.40995600	1.74677500
C	-4.16174500	-1.90653200	0.98848300
C	-3.55686200	-0.67509400	0.73709500
O	-4.45630400	0.34148300	0.94590600
C	-2.24797900	-0.32428800	0.32734300
C	-1.86859300	1.02983200	0.13643800
C	-0.59920100	1.35606700	-0.25990000
C	0.37799200	0.34343100	-0.49222700
C	-0.00139000	-1.01068700	-0.30130600
C	-1.27077300	-1.33692100	0.09506200
C	1.68685800	0.69423400	-0.90203600
O	2.58617700	-0.32236700	-1.11125900
C	3.75639500	0.25044900	-1.49283700
C	3.62273200	1.65761500	-1.53416800
C	2.29181300	1.92568600	-1.15318200
C	4.92029000	-0.41815600	-1.80096000
C	6.01196100	0.37104600	-2.17164000
C	5.91691800	1.77114000	-2.22407800
C	4.74103400	2.42909300	-1.91175600
H	-6.85093400	1.51834600	1.59044700
H	-8.82197800	0.12781000	2.25775400
H	-8.65961000	-2.32663900	2.35175400
H	-6.54774300	-3.49183000	1.79066900
H	-3.68460100	-2.87075200	0.90241100
H	-2.60137700	1.80930400	0.30951200
H	-0.33479300	2.39853200	-0.39862200
H	0.73139300	-1.79016000	-0.47438600
H	-1.53518400	-2.37938600	0.23377400
H	1.81478200	2.88992700	-1.06673300
H	4.98057600	-1.49927600	-1.75657500
H	6.95162200	-0.10873900	-2.42387300
H	6.78947800	2.34575400	-2.51712200
H	4.67782900	3.51098700	-1.95530900

5Od compound

C	0.77190100	1.33101800	0.31960600
C	1.62079700	0.23573900	0.12600800
C	1.05280300	-1.05403900	-0.15589700
C	-0.30957500	-1.34282300	-0.26152600
C	-1.15847000	-0.24753600	-0.06797000
C	-0.59047700	1.04223500	0.21397200
C	-2.56996500	-0.04436600	-0.07527500
C	-2.76916600	1.32119400	0.19568600
O	-1.55436300	1.96141500	0.36778400
C	3.03229600	0.03259500	0.13318200
C	3.23149500	-1.33297700	-0.13772300
O	2.01668800	-1.97321900	-0.30971000
C	-3.70008400	-0.85133400	-0.27844000
C	-4.96171300	-0.25669500	-0.20092000
C	-5.11783900	1.09903400	0.06955200
C	-3.99404600	1.92794100	0.27692200
C	4.16242300	0.83960200	0.33615400
C	5.42405400	0.24497800	0.25856200
C	5.58017700	-1.11076400	-0.01184900
C	4.45637900	-1.93970200	-0.21906500
H	1.12289700	2.33164900	0.53522800
H	-0.66057100	-2.34345100	-0.47716300
H	-3.60026400	-1.91007500	-0.49042700
H	-5.84348200	-0.86976500	-0.35604900
H	-6.11139800	1.52909700	0.12282200
H	-4.09003500	2.98597100	0.48887800
H	4.06260600	1.89835600	0.54808100
H	6.30582700	0.85807200	0.41356200
H	6.57373900	-1.54081200	-0.06519900
H	4.55236600	-2.99774000	-0.43098600

5Sa compound

C	0.79926200	1.41239100	-0.07683300
C	-0.43466300	1.43495500	-0.67181400
C	-1.00512500	0.26924600	-1.24926300
C	-0.23704000	-0.92269000	-1.18210800
C	0.99684000	-0.94527900	-0.58703300
C	1.56718000	0.22036500	-0.00933500
C	-2.28692300	0.28658000	-1.86793700
C	2.84838700	0.20271700	0.61055200
C	-2.98474800	-0.76332200	-2.47817800
C	-4.22470100	-0.39339900	-2.98434400
C	-4.54312900	0.95121500	-2.79118200
C	3.54700300	1.25303300	1.21917300
C	4.78548800	0.88233200	1.72835600
C	5.10192900	-0.46333000	1.53927200
C	-5.73121300	1.66026100	-3.18450200
C	6.28810900	-1.17338300	1.93650500
C	-5.89659400	3.03434200	-2.90807800
C	-7.04335600	3.70722100	-3.29069000
C	-8.06575400	3.03891800	-3.96107000
C	-7.92077300	1.68029700	-4.24334400
C	-6.77831400	1.00044000	-3.86467200
C	6.45035000	-2.54912000	1.66653100
C	7.59528400	-3.22296500	2.05290100
C	8.61890000	-2.55402200	2.72077700
C	8.47701100	-1.19377000	2.99669900
C	7.33640200	-0.51293500	2.61422600
S	-3.24097000	1.75176900	-1.95228400
S	3.79987600	-1.26382400	0.70015200
H	1.19172600	2.32827100	0.35000200
H	-0.98703600	2.36918400	-0.70045200
H	-0.62957200	-1.83860700	-1.60880100
H	1.54924800	-1.87948900	-0.55847000
H	-2.59116800	-1.76917900	-2.54725100
H	-4.88816300	-1.08642000	-3.48548000
H	3.15508400	2.25976600	1.28483700
H	5.44924100	1.57550400	2.22889700
H	-5.11301900	3.57564200	-2.38660500
H	-7.14290800	4.76409200	-3.06463700
H	-8.96395900	3.56852300	-4.26008300
H	-8.70991300	1.14813300	-4.76504200
H	-6.69053300	-0.05509700	-4.09617200
H	5.66567900	-3.09099600	1.14731100
H	7.69241200	-4.28111400	1.83182500
H	9.51566700	-3.08438700	3.02274700
H	9.26715900	-0.66107600	3.51632400
H	7.25112100	0.54392000	2.84058900

5Sb compound

C	-5.64942400	-1.37058300	1.39951500
C	-6.03378700	-0.00060600	1.43797300
C	-7.31321100	0.39104600	1.79843500
C	-8.23964000	-0.59417800	2.13016900
C	-7.88573800	-1.95316500	2.10011700
C	-6.61441200	-2.34720700	1.74222300
C	-4.30941000	-1.53880800	1.00849300
C	-3.64052800	-0.34072200	0.74194200
S	-4.70890900	1.03751000	0.98420700
C	-2.29149400	-0.15826800	0.32930700
C	-1.74285300	1.12947900	0.09222500
C	-0.44288600	1.29605400	-0.30431700
C	0.42061700	0.17722400	-0.49718700
C	-0.12806600	-1.11053200	-0.26024700
C	-1.42807100	-1.27711400	0.13617000
C	1.76991200	0.35973400	-0.90894300
S	2.83979300	-1.01820500	-1.14619700
C	4.16457200	0.01990000	-1.60027900
C	3.77900200	1.38964500	-1.56584900
C	2.43818100	1.55770700	-1.17753200
C	5.44493900	-0.37156500	-1.95758200
C	6.37111200	0.61361600	-2.29015800
C	6.01599300	1.97236900	-2.26417000
C	4.74372200	2.36622400	-1.90944100
H	-7.59011900	1.43961900	1.82270800
H	-9.24611400	-0.30634100	2.41486600
H	-8.62679300	-2.70081000	2.36318800
H	-6.34531600	-3.39844100	1.72038500
H	-3.83567000	-2.50814500	0.92069000
H	-2.36696800	2.00767100	0.22774900
H	-0.06891700	2.29904800	-0.47290300
H	0.49605200	-1.98872200	-0.39576300
H	-1.80195300	-2.28009100	0.30505000
H	1.96334000	2.52683200	-1.09340900
H	5.72276400	-1.41996200	-1.97879500
H	7.37832400	0.32592500	-2.57238500
H	6.75686200	2.71998300	-2.52785200
H	4.47369500	3.41727900	-1.89070900

5Sd compound

C	1.28670800	0.05783400	0.61239500
C	2.66331000	0.05868100	0.99815000
C	3.53091000	-0.24057000	-0.08206900
C	1.10139400	-0.24275100	-0.76600100
C	-0.14111200	-0.30685600	-1.39380500
C	-1.28670800	-0.05783400	-0.61239500
C	-1.10139400	0.24275100	0.76600100
C	0.14111200	0.30685600	1.39380500
C	3.24787000	0.30576200	2.25109400
C	4.63308100	0.24921000	2.38585900
C	5.46317500	-0.04751700	1.30645300
C	4.90598300	-0.29832000	0.04467800
C	-2.66331000	-0.05868100	-0.99815000
C	-3.53091000	0.24057000	0.08206900
C	-3.24787000	-0.30576200	-2.25109400
C	-4.63308100	-0.24921000	-2.38585900
C	-5.46317500	0.04751700	-1.30645300
C	-4.90598300	0.29832000	-0.04467900
H	-0.22355700	-0.54066200	-2.44886900
H	0.22355700	0.54066200	2.44886900
H	2.62620000	0.53912500	3.10872800
H	5.07655900	0.44149700	3.35778000
H	6.53819400	-0.08519000	1.43854200
H	5.53711900	-0.53073100	-0.80610700
H	-2.62620000	-0.53912500	-3.10872800
H	-5.07655900	-0.44149700	-3.35778000
H	-6.53819400	0.08519000	-1.43854200
H	-5.53711900	0.53073100	0.80610700
S	2.61865200	-0.51607400	-1.55157200
S	-2.61865200	0.51607400	1.55157200

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