Electronic Supplementary Information

A DFT/ TDDFT Mission to Probe Push-Pull Vinyl Coupled Thiophene Oligomers for Optoelectronic Applications

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SIT1: Selected geometrical parameters of VCTOs optimized at B3LYP/6-31g(d) level.

Molecules	Bonds			Angle(°)	Torsional angle
	C-C	C=C	C-S	C-C-C	
VCTO1	1.43/1.44/1.42/1.42 (1.44/1.42)	1.37/1.38/1.40 (1.38/1.40)	1.75/1.74/1.75 (1.75/1.74)	130/131/130 (130)	178/-180 (179)
VCTO1a	1.44/1.43/1.44/1.44	1.35/1.39/1.38	1.75/175/1.76	131/129/129	-177/178
VCTO1b	1.44/1.44/1.41/1.44	1.36/1.38/1.38	1.75/1.75/1.76	129/127/128	-176/176
VCTO1c	1.44/1.46/1.43/1.44	1.35/1.36/1.38	1.75/1.76/1.75	129/127/128	-177/157
VCTO2	1.42/1.43/1.43/1.43 (1.43/1.42)	1.37/1.39/1.38 (1.38/1.37)	1.75/1.75/1.75 (1.75/1.74)	128/130/127 (130)	-180/180 (180)
VCTO2a	1.44/1.44/1.44/1.44	1.35/1.38/1.38	1.75/1.75/1.75	127/129/130	-180/-180
VCTO2b	1.44/1.43/1.44/1.43	1.35/1.35/1.38	1.75/1.75/1.75	129/129/121	-167/170
VCTO2c	1.44/1.44/1.44/1.44	1.35/1.35/1.38	1.75/1.75/1.75	129/129/128	-166/-168
VCTO3	1.43/1.43/1.43/1.43 (1.43/1.43)	1.37/1.39 (1.39/1.39)	1.75/1.75 (1.74/1.75)	122/129/130 (122)	-177/178 (179)
VCTO3a	1.43/1.43/1.42/1.43	1.36/1.39/1.39	1.75/1.76	124/126/127	-176/177
VCTO3b	1.39/1.43/1.43	1.36/1.36/1.39	1.75/1.75	126/134/135	-180/179
VCTO3c	1.44/1.43/1.40	1.36/1.39/1.39	1.75/1.76	122/126/125	-180/180
VCTO4ew	1.45/1.45/1.44/1.44	1.34/1.38/1.38	1.75/1.76/1.75	127/129/131	-171/170
VCTO4a	1.44/1.43/1.4/1.39	1.37/1.37/1.38	1.76/1.75/1.75	128/131/129	179/180
VCTO4b	1.44/1.39/1.43/1.44	1.37/1.38/1.36	1.76/1.76/1.76	128/136/131	168/170
VCTO4c	1.44/1.44/1.44/1.43	1.37/1.37/1.38	1.75/1.75/1.76	128/131/129	173/170
VCTO4er	1.44/1.38/1.44/1.43	1.37/1.38/1.38	1.75/1.75/1.75	128/132/129	173/175

Values in parentheses are experimentally reported bond parameters.

SIT2: HOMO and LUMO energy levels of VCTOs calculated at B3LYP/6-31g (d) level.

Molecules	HOMO(eV)	LUMO(eV)	E_{HOMO}- E_{LUMO} (eV)
VCTO 1	-5.51	-3.19	2.32 (1.91)
VCTO1a	-4.67	-2.31	2.36
VCTO1b	-4.72	-2.64	2.08
VCTO1c	-4.63	-2.20	2.43
VCTO2	-5.64	-3.40	2.23 (1.89)
VCTO2a	-4.90	-2.58	2.32
VCTO2b	-4.98	-2.83	2.15
VCTO2c	-4.86	-2.43	2.42
VCTO3	-7.11	-4.08	3.03 (2.78)
VCTO3a	-5.31	-2.45	2.85
VCTO3b	-5.14	-2.27	2.86
VCTO3c	-4.73	-1.57	3.16
VCTO4ew	-5.13	-2.91	2.22
VCTO4a	-4.49	-2.78	1.71
VCTO4b	-4.53	-3.02	1.50
VCTO4c	-4.41	-2.36	2.04
VCTO4er	-4.31	-1.80	2.51

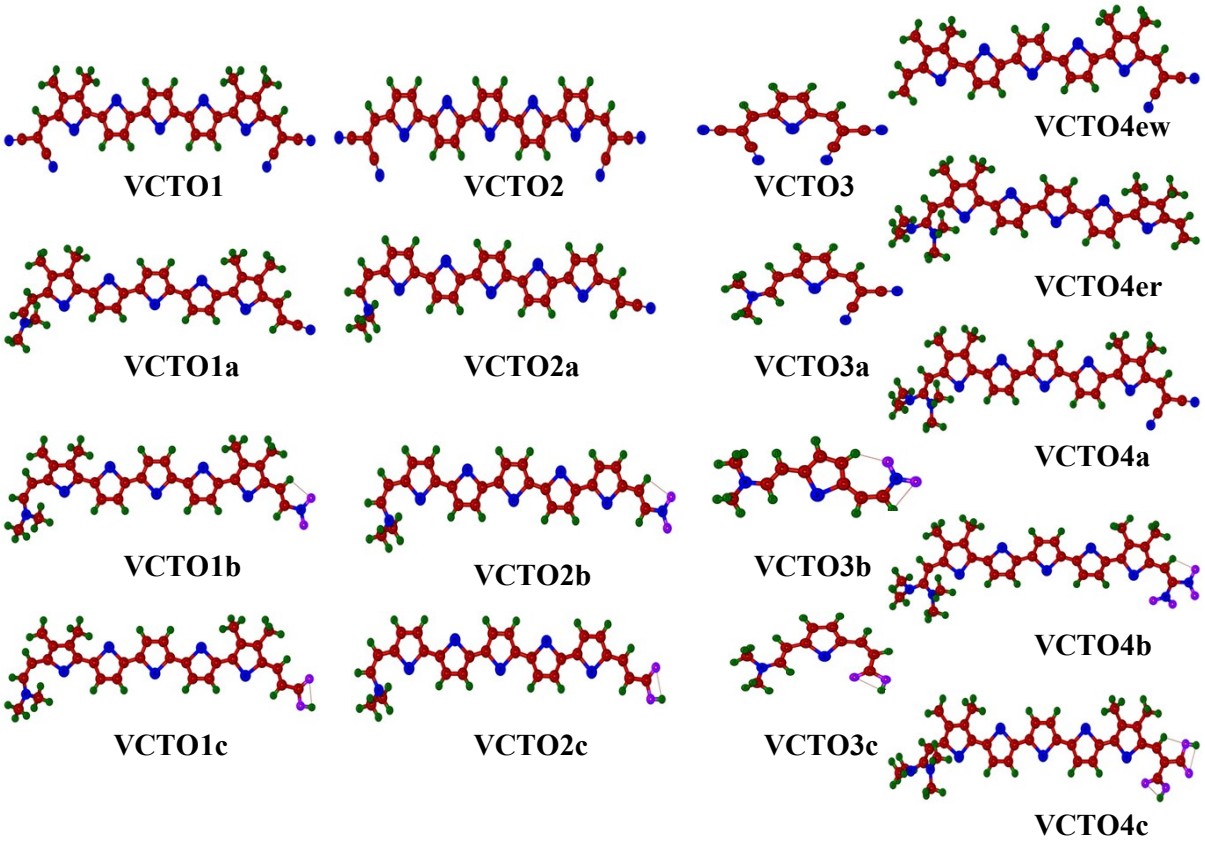
Values in parentheses are obtained from experiments. (Band gap reported in solution phase).

SIT3: B3LYP/6-31g(d) natural charges at donor and acceptor segments of VCTOs.

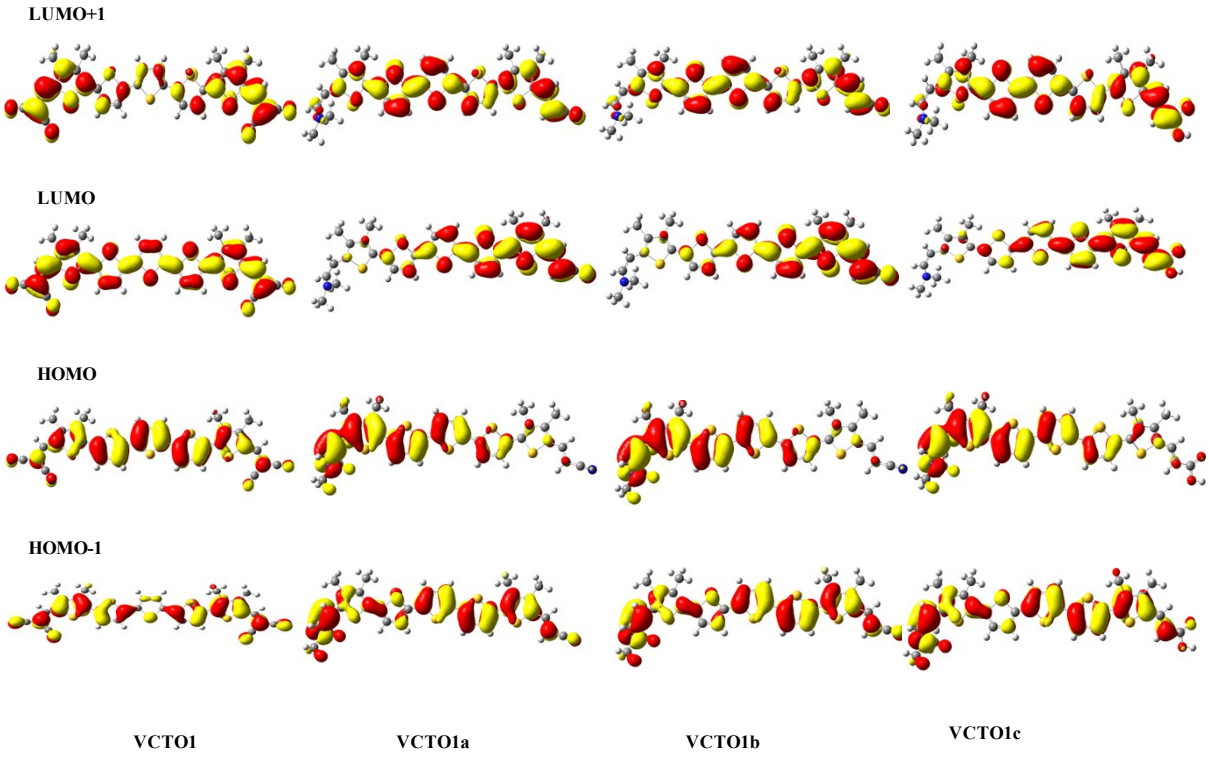
Molecules	Donor	Acceptor
VCTO 1	-	-0.638
VCTO1a	0.235	-0.158
VCTO1b	0.237	-0.198
VCTO1c	0.234	-0.151
VCTO2	-	-0.616
VCTO2a	0.069	-0.151
VCTO2b	0.068	-0.189
VCTO2c	0.063	-0.152
VCTO3	-	-0.692
VCTO3a	0.336	-0.376
VCTO3b	0.288	-0.243
VCTO3c	0.264	-0.204
VCTO4ew	0.03	-0.323
VCTO4a	0.291	-0.346
VCTO4b	0.294	-0.366
VCTO4c	0.288	-0.293
VCTO4 er	0.278	-

SIT4: Calculated absorption maxima using different functional with 6-31g(d) basis set.

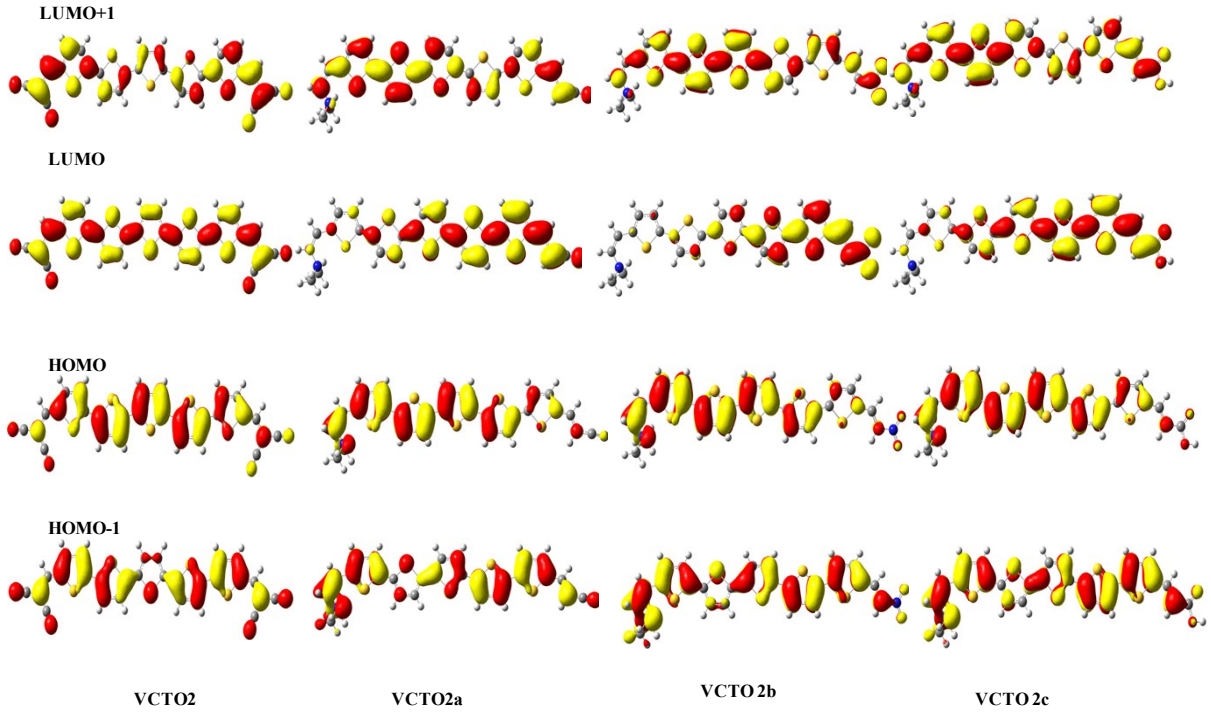
Molecule	Functional	Wavelength (λ_{max}) nm	Exp Wavelength (λ_{max}) nm
VCTO1	B3LYP	641	**527**
	B1LYP	615	
	CAM-B3LYP	513	
	PBE	608	
	M062X	**513**	
VCTO2	B3LYP	582	**530**
	B1LYP	557	
	CAM-B3LYP	473	
	PBE	551	
	M062X	**532**	
VCTO3	B3LYP	427	**406**
	B1LYP	421	
	CAM-B3LYP	399	
	PBE	418	
	M062X	**394**	



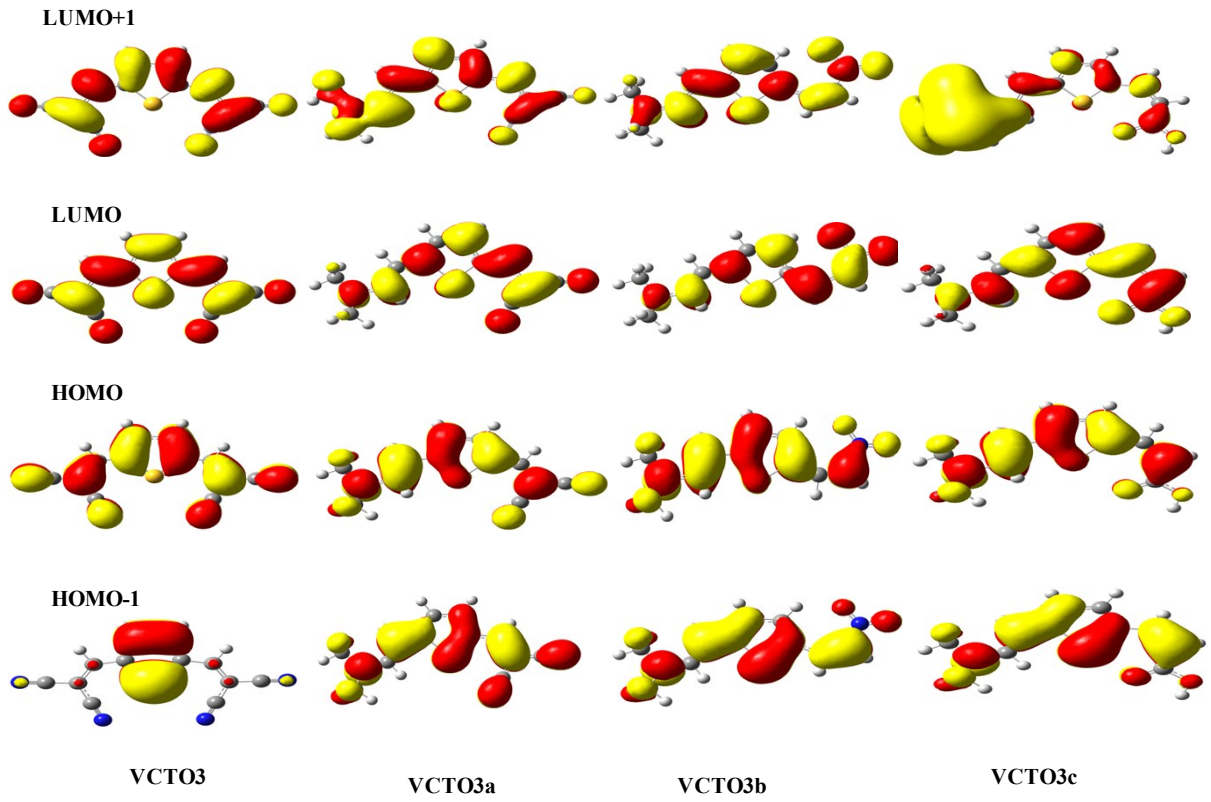
SIF1: Structure of experimentally reported and designed VCTOs.



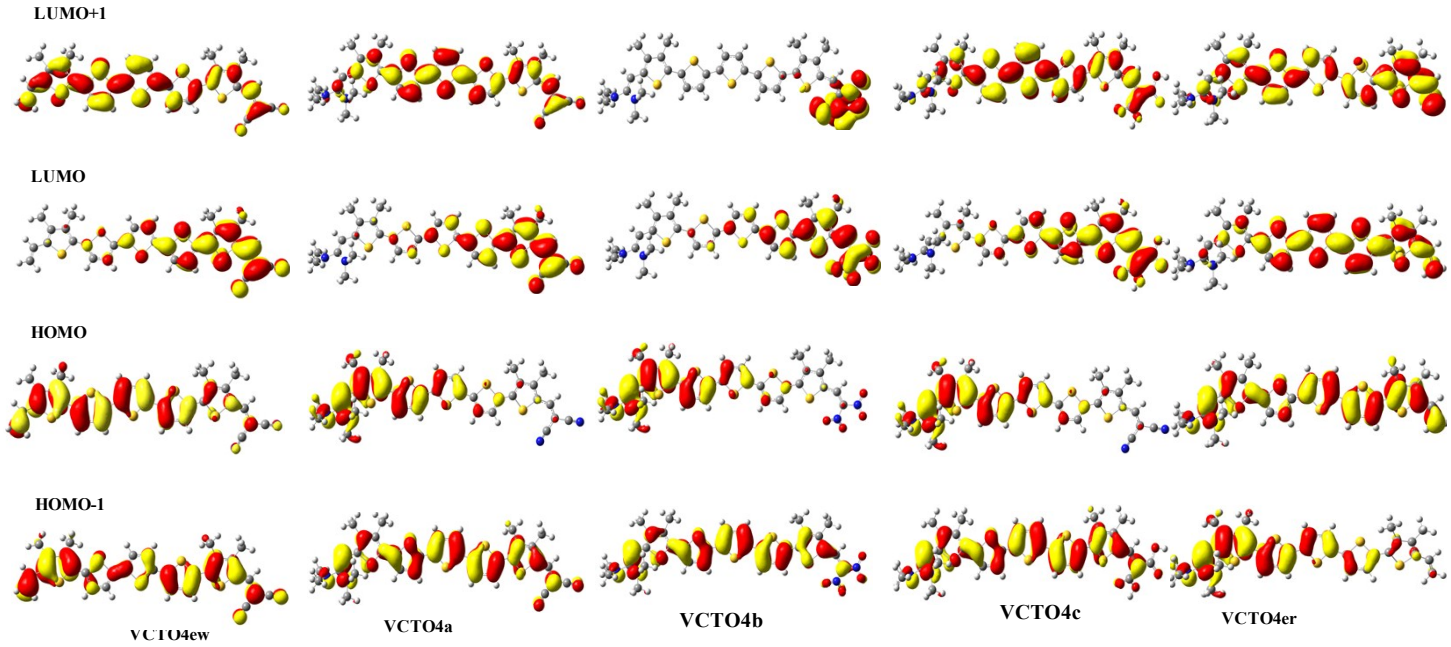
SIF2: Frontier molecular orbitals of VCTO1s.



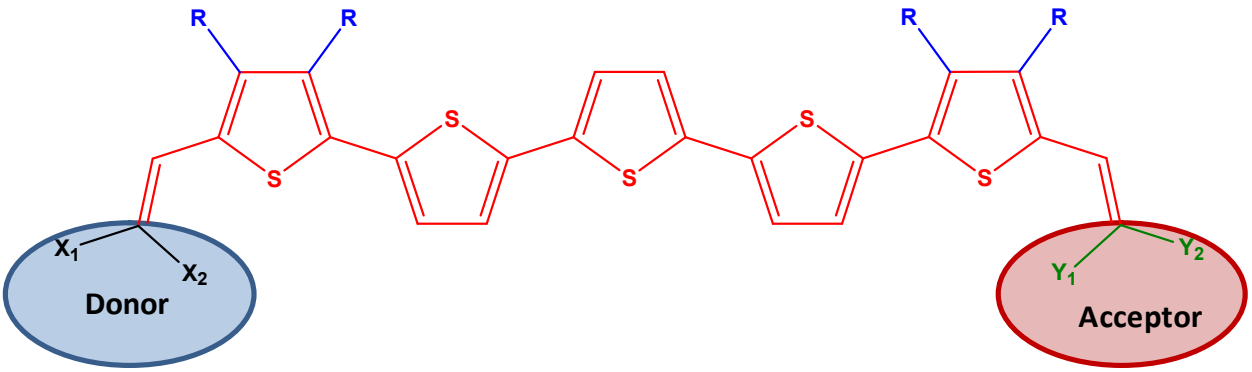
SIF3: Frontier molecular orbitals of VCTO2s.



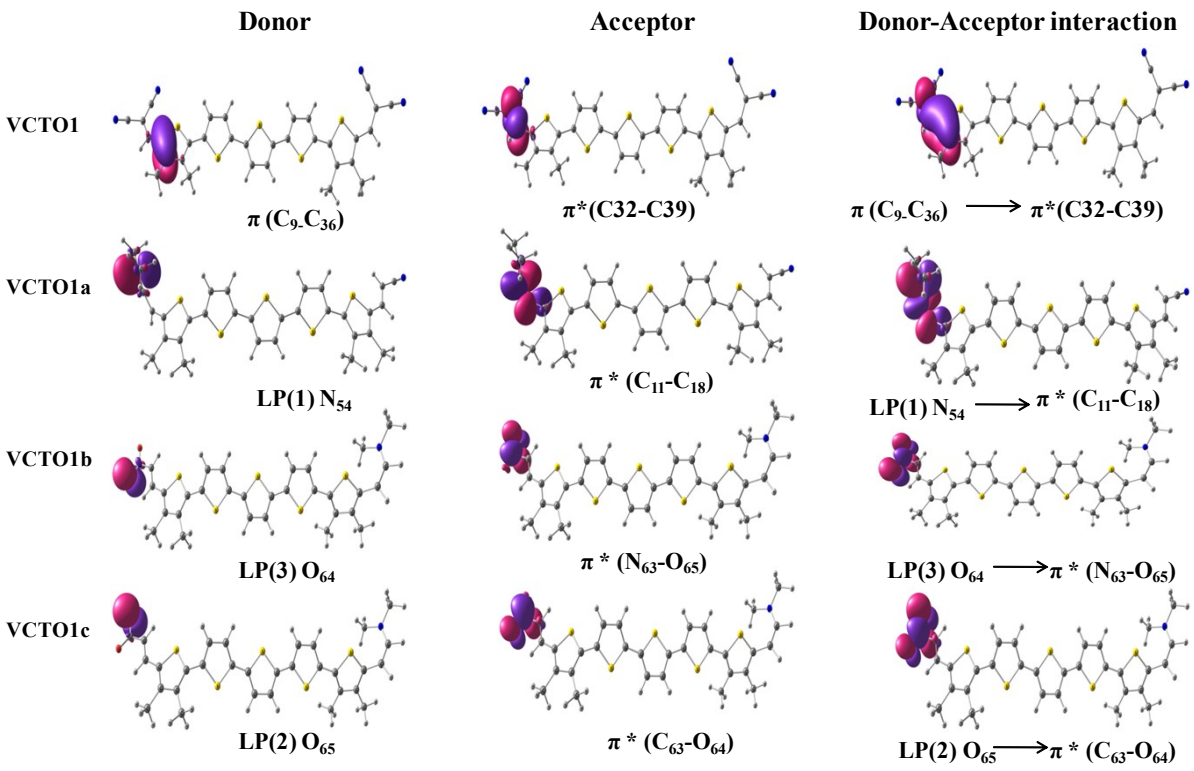
SIF4: Frontier molecular orbitals of VCTO3s.



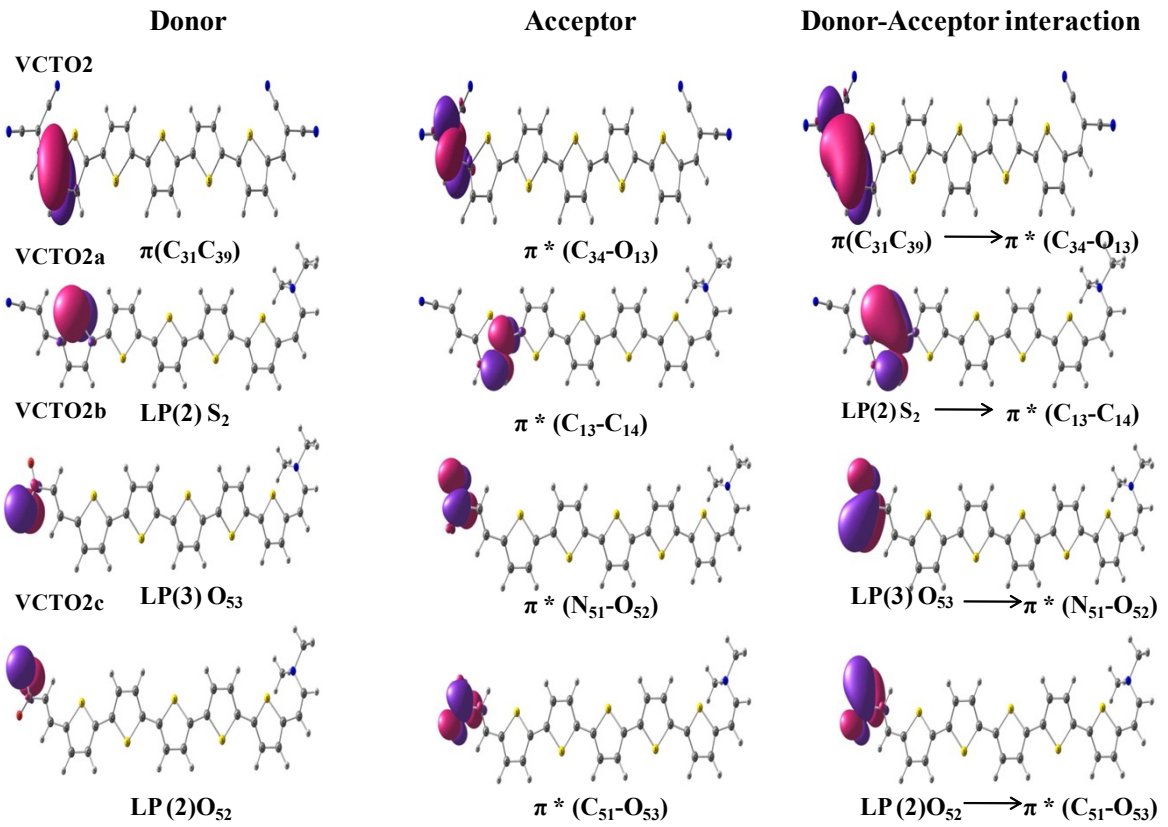
SIF5: Frontier molecular orbitals of VCTO4s.



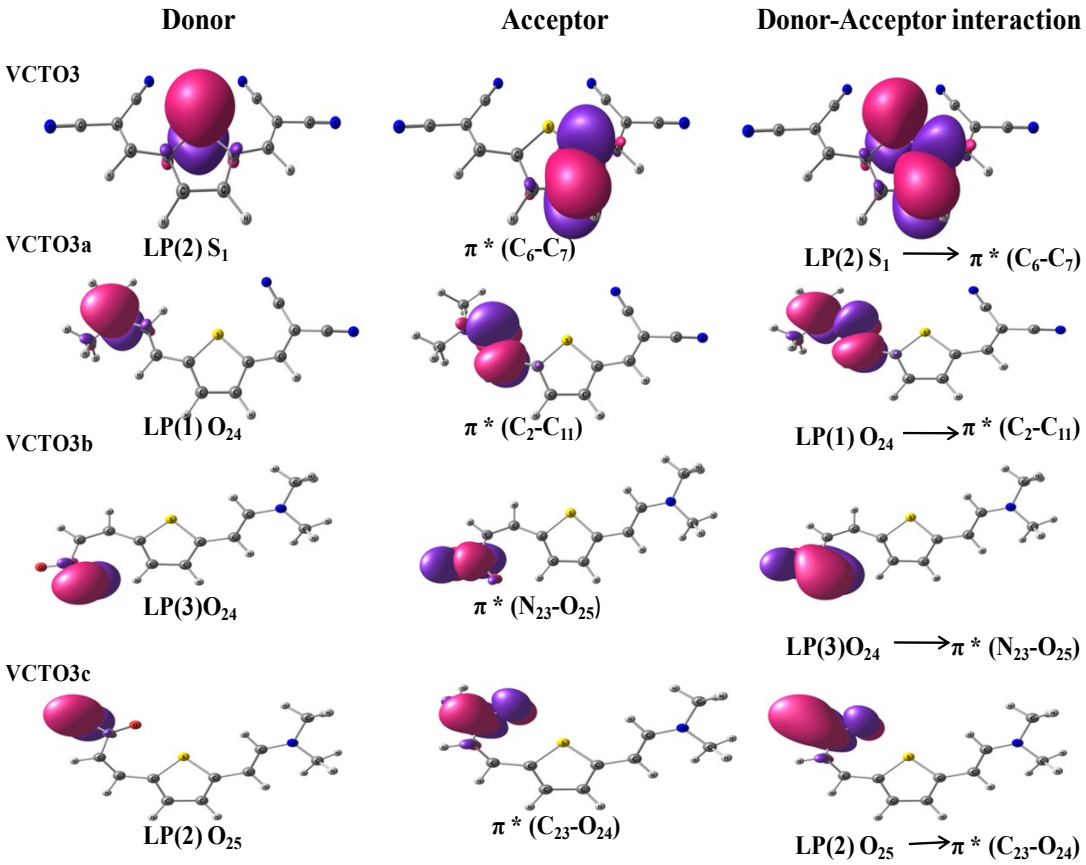
SIF6: Donor and Acceptor moieties of VCTOs used for the calculation of NBO charges.



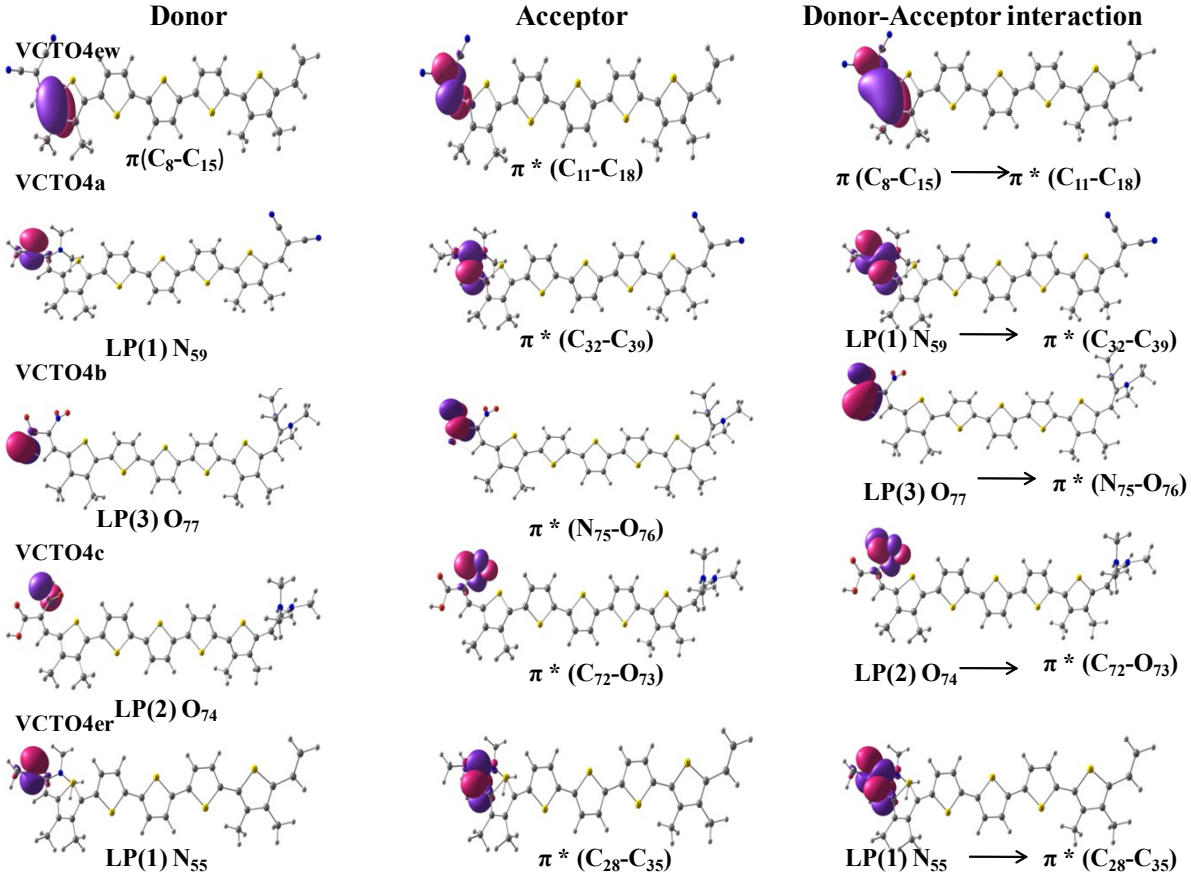
SIF7: Projections of donor, acceptor, donor-acceptor interactions in VCTO1s.



SIF8: Projections of donor, acceptor, donor-acceptor interactions in VCTO2s.



SIF9: Projections of donor, acceptor, donor-acceptor interactions in VCTO3s.



SIF10: Projections of donor, acceptor, donor-acceptor interactions in VCTO4s.

XYZ coordinates of optimized geometry

Molecule name:1_a

S	-0.33123	-0.77267	0.41114
S	7.30257	-0.83834	-0.60349
S	3.51444	1.27210	-0.30296
C	0.89976	0.46820	0.22504
C	2.30054	0.12566	0.24235
C	4.83348	0.16915	0.07486
C	0.30528	1.70571	0.06308
C	8.69018	0.23014	-0.71296
C	2.90865	-1.04305	0.65801
H	2.35211	-1.88662	1.05326
C	9.98954	-0.25910	-1.16657
H	10.42247	0.30269	-1.99197
C	6.22080	0.48572	-0.19740
C	6.90664	1.69071	-0.19754
C	8.30153	1.54087	-0.49924
C	4.31841	-1.01926	0.56276
H	4.95265	-1.84452	0.86721
C	10.73385	-1.32805	-0.77389
S	-7.98694	-1.18928	-0.18099
S	-4.30732	1.09825	-0.02736
C	-1.63063	0.40739	0.30082
C	-3.00992	-0.00135	0.40400
C	-5.54384	-0.08011	0.39827
C	-1.10737	1.67093	0.10608
C	-9.42026	-0.18160	-0.19227
C	-3.53263	-1.21083	0.82397
H	-2.91175	-2.03573	1.15656
C	-10.72349	-0.72602	-0.46178
H	-11.53801	-0.00774	-0.50032
C	-6.96019	0.17227	0.22825
C	-7.69869	1.34385	0.32553
C	-9.09449	1.14166	0.08086
C	-4.94449	-1.25418	0.81694
H	-5.51722	-2.11731	1.13885
C	-11.03120	-2.03094	-0.67049
H	-1.72750	2.55705	0.01917

H	0.87661	2.61955	-0.05953
C	-10.08464	2.27403	0.14562
H	-9.78027	3.09891	-0.50954
H	-11.08978	1.97097	-0.15368
H	-10.15534	2.68151	1.16242
C	-7.13362	2.69395	0.68410
H	-6.20976	2.60620	1.26086
H	-6.90854	3.29367	-0.20830
H	-7.84638	3.26804	1.28498
C	6.29796	3.03204	0.11944
H	5.99398	3.56702	-0.79091
H	5.41335	2.94058	0.75505
H	7.01703	3.67351	0.63974
C	9.26214	2.69976	-0.55202
H	10.28507	2.35097	-0.71557
H	9.01051	3.40227	-1.35758
H	9.25736	3.27400	0.38369
N	10.65071	-2.15237	0.32173
C	9.78186	-1.89173	1.45212
C	11.24667	-3.47444	0.26106
H	10.26470	-2.27045	2.36130
H	9.63005	-0.81600	1.55631
H	8.79527	-2.36952	1.36024
H	11.68282	-3.73503	1.23314
H	12.04185	-3.48882	-0.49038
H	10.51478	-4.25428	-0.00356
C	-12.35946	-2.46075	-0.93607
N	-13.44367	-2.82906	-1.15562
H	-10.27226	-2.80916	-0.64059
H	11.59835	-1.56664	-1.39258

Molecule name: 1_b

S	-0.053733000	0.754438000	-0.245153000
S	-7.788586000	0.547648000	-0.682543000
S	-3.946027000	-1.329905000	0.106792000
C	-1.305243000	-0.477038000	-0.156207000
C	-2.699178000	-0.112244000	-0.118397000
C	-5.231403000	-0.126965000	0.077851000
C	-0.730970000	-1.735026000	-0.132676000

C	-9.154889000	-0.387671000	-0.101999000
C	-3.276669000	1.138915000	-0.221567000
H	-2.696865000	2.045345000	-0.362564000
C	-10.513001000	-0.113998000	-0.563631000
H	-11.037043000	-0.978750000	-0.965790000
C	-6.634648000	-0.477070000	0.158072000
C	-7.288186000	-1.512519000	0.808868000
C	-8.713321000	-1.461907000	0.650672000
C	-4.685031000	1.130451000	-0.113383000
H	-5.293632000	2.026800000	-0.158522000
C	-11.225637000	1.043327000	-0.627064000
S	7.632678000	0.978820000	0.162569000
S	3.893756000	-1.233410000	-0.130294000
C	1.225236000	-0.452984000	-0.269298000
C	2.609261000	-0.059440000	-0.351521000
C	5.143766000	-0.024287000	-0.406781000
C	0.680481000	-1.720713000	-0.195654000
C	9.039709000	-0.055334000	0.016553000
C	3.146294000	1.190982000	-0.603169000
H	2.534727000	2.067380000	-0.788510000
C	10.363543000	0.428098000	0.271656000
H	11.178594000	-0.286704000	0.206301000
C	6.557510000	-0.318091000	-0.320769000
C	7.263065000	-1.493612000	-0.557074000
C	8.670309000	-1.343435000	-0.360473000
C	4.556797000	1.209242000	-0.630684000
H	5.137455000	2.101994000	-0.836820000
C	10.716366000	1.690687000	0.588992000
H	1.284424000	-2.622148000	-0.203223000
H	-1.315865000	-2.647219000	-0.083622000
C	9.634198000	-2.480254000	-0.570402000
H	9.642529000	-2.803102000	-1.619300000
H	10.658602000	-2.214975000	-0.302967000
H	9.349781000	-3.351160000	0.031831000
C	6.644079000	-2.792328000	-1.005870000
H	6.348629000	-3.421526000	-0.155379000
H	5.750875000	-2.625574000	-1.613845000
H	7.349387000	-3.374174000	-1.606769000
C	-6.612594000	-2.574316000	1.637115000
H	-6.410439000	-3.481153000	1.050483000
H	-5.658628000	-2.230532000	2.045588000
H	-7.245474000	-2.874957000	2.478629000
C	-9.648696000	-2.467815000	1.268849000

H	-9.491793000	-2.555806000	2.351677000
H	-10.691062000	-2.178175000	1.112280000
H	-9.508833000	-3.471103000	0.844676000
N	-11.020971000	2.280908000	-0.068056000
C	-9.997562000	2.549577000	0.922643000
C	-11.657879000	3.441462000	-0.663680000
H	-10.360564000	3.332378000	1.599719000
H	-9.802468000	1.645771000	1.502482000
H	-9.047060000	2.886131000	0.482892000
H	-11.961631000	4.146209000	0.119867000
H	-12.550195000	3.132297000	-1.216159000
H	-10.992798000	3.974416000	-1.361768000
N	12.098154000	2.024493000	0.821744000
O	12.960510000	1.142364000	0.728816000
O	12.331120000	3.205445000	1.105834000
H	10.062089000	2.544690000	0.697046000
H	-12.169701000	0.997742000	-1.169005000

Molecule name : 1_c

S	-0.057997000	0.739687000	-0.278578000
S	-7.793456000	0.545753000	-0.685919000
S	-3.956243000	-1.328155000	0.120459000
C	-1.312734000	-0.486022000	-0.153692000
C	-2.705869000	-0.116036000	-0.114777000
C	-5.237964000	-0.121079000	0.088163000
C	-0.741700000	-1.744018000	-0.106227000
C	-9.162529000	-0.376700000	-0.091183000
C	-3.279541000	1.136023000	-0.224321000
H	-2.697051000	2.039729000	-0.371450000
C	-10.520007000	-0.105954000	-0.558326000
H	-11.043346000	-0.972809000	-0.957049000
C	-6.642619000	-0.466958000	0.173174000
C	-7.298855000	-1.489729000	0.840276000
C	-8.724138000	-1.438864000	0.679419000
C	-4.688235000	1.132742000	-0.112334000
H	-5.294104000	2.030801000	-0.161367000
C	-11.231858000	1.051055000	-0.629292000
S	7.624376000	0.947430000	0.135633000
S	3.886242000	-1.245198000	-0.102333000
C	1.217395000	-0.471536000	-0.285856000

C	2.602650000	-0.083271000	-0.387965000
C	5.137508000	-0.056915000	-0.450669000
C	0.670089000	-1.735323000	-0.179844000
C	9.033160000	-0.087062000	0.010516000
C	3.141430000	1.149589000	-0.707005000
H	2.530980000	2.015285000	-0.940741000
C	10.355812000	0.406988000	0.280196000
H	11.164997000	-0.317992000	0.228305000
C	6.552448000	-0.352057000	-0.350062000
C	7.259060000	-1.526427000	-0.573442000
C	8.666749000	-1.374618000	-0.362707000
C	4.553568000	1.163372000	-0.738572000
H	5.136974000	2.041380000	-0.994022000
C	10.714732000	1.672659000	0.592796000
H	1.271945000	-2.638092000	-0.173237000
H	-1.328406000	-2.653453000	-0.032155000
C	9.629568000	-2.515490000	-0.558259000
H	9.652154000	-2.840080000	-1.606686000
H	10.650695000	-2.252611000	-0.276213000
H	9.333829000	-3.385700000	0.039971000
C	6.650355000	-2.828969000	-1.024634000
H	6.429733000	-3.493286000	-0.177941000
H	5.716028000	-2.672754000	-1.569474000
H	7.334015000	-3.370116000	-1.686703000
C	-6.626887000	-2.538746000	1.687549000
H	-6.439281000	-3.461279000	1.120871000
H	-5.665927000	-2.195369000	2.079427000
H	-7.255532000	-2.812929000	2.541367000
C	-9.662041000	-2.432864000	1.312740000
H	-9.505399000	-2.504984000	2.396802000
H	-10.703646000	-2.143002000	1.151304000
H	-9.524482000	-3.442859000	0.903898000
N	-11.027007000	2.292322000	-0.077360000
C	-10.000565000	2.566964000	0.908576000
C	-11.657701000	3.449699000	-0.685357000
H	-10.360272000	3.356176000	1.580008000
H	-9.806007000	1.667624000	1.495446000
H	-9.050320000	2.897702000	0.463811000
H	-11.957402000	4.164397000	0.090726000
H	-12.551992000	3.139418000	-1.234101000
H	-10.990253000	3.971874000	-1.389483000
C	12.126587000	1.988489000	0.840929000
O	13.061631000	1.207825000	0.798621000

O	12.301194000	3.306451000	1.137789000
H	13.258833000	3.416008000	1.284504000
H	10.001389000	2.487590000	0.668933000
H	-12.175645000	1.002965000	-1.171562000

Molecule name : 1

S	0.000082000	0.772118000	-0.001433000
S	-7.705796000	0.858101000	-0.170727000
S	-3.913308000	-1.282587000	0.202591000
C	-1.261883000	-0.447311000	0.077058000
C	-2.649968000	-0.068346000	0.159386000
C	-5.178154000	-0.063187000	0.317418000
C	-0.704326000	-1.712714000	0.042416000
C	-9.084500000	-0.183085000	0.139279000
C	-3.203253000	1.199128000	0.225320000
H	-2.606766000	2.105049000	0.223808000
C	-10.435866000	0.213440000	-0.062762000
H	-11.173926000	-0.556423000	0.139110000
C	-6.587260000	-0.382537000	0.340660000
C	-7.251186000	-1.552229000	0.713806000
C	-8.663699000	-1.440187000	0.595578000
C	-4.609441000	1.200963000	0.311233000
H	-5.199224000	2.108214000	0.384966000
C	-10.969645000	1.413862000	-0.472473000
N	-13.546303000	1.631374000	-0.693782000
C	-12.389540000	1.540007000	-0.596399000
C	-10.201524000	2.575214000	-0.789597000
N	-9.587293000	3.529999000	-1.050999000
S	7.705372000	0.858227000	0.170899000
S	3.913613000	-1.282575000	-0.202166000
C	1.261992000	-0.447327000	-0.080443000
C	2.650084000	-0.068382000	-0.162873000
C	5.178318000	-0.063324000	-0.319645000
C	0.704410000	-1.712722000	-0.046012000
C	9.084471000	-0.183006000	-0.137209000
C	3.203251000	1.198983000	-0.231673000
H	2.606632000	2.104818000	-0.233001000
C	10.435626000	0.213633000	0.066073000
H	11.173893000	-0.556356000	-0.134569000
C	6.587487000	-0.382656000	-0.341281000

C	7.251843000	-1.552438000	-0.713263000
C	8.664231000	-1.440305000	-0.593449000
C	4.609507000	1.200769000	-0.316850000
H	5.199262000	2.107866000	-0.392677000
C	10.968954000	1.414289000	0.475657000
N	13.545367000	1.631953000	0.699661000
C	12.388713000	1.540518000	0.601066000
C	10.200473000	2.575826000	0.791239000
N	9.585948000	3.530772000	1.051358000
H	1.297819000	-2.620024000	-0.084730000
H	-1.297770000	-2.620013000	0.080649000
C	9.585470000	-2.576950000	-0.949735000
H	9.523747000	-2.812979000	-2.019582000
H	10.632015000	-2.364782000	-0.725665000
H	9.312245000	-3.486402000	-0.402377000
C	6.571011000	-2.799327000	-1.216717000
H	6.195359000	-3.421929000	-0.393813000
H	5.718754000	-2.561034000	-1.860075000
H	7.259717000	-3.416216000	-1.799807000
C	-6.569575000	-2.798917000	1.216714000
H	-6.191439000	-3.419721000	0.393601000
H	-5.718863000	-2.560368000	1.862066000
H	-7.258475000	-3.417681000	1.797545000
C	-9.584579000	-2.576685000	0.953291000
H	-9.520862000	-2.813051000	2.022938000
H	-10.631488000	-2.364117000	0.731337000
H	-9.312721000	-3.486053000	0.405106000

Molecule name: 2_a

S	0.331824000	0.642614000	-0.028725000
S	8.166837000	0.917817000	-0.023289000
S	4.321111000	-1.280195000	0.027753000
C	1.638906000	-0.530873000	0.063699000
C	3.014681000	-0.105555000	0.058240000
C	5.544354000	-0.016350000	0.041799000
C	1.121853000	-1.811122000	0.132387000
C	9.471473000	-0.259007000	-0.006329000
C	3.530145000	1.178838000	0.070502000
H	2.903854000	2.064139000	0.093265000
C	10.863425000	0.092497000	-0.033851000

H	11.546364000	-0.755021000	-0.022372000
C	6.946222000	-0.344792000	0.031414000
C	7.545978000	-1.593557000	0.057581000
H	6.979843000	-2.517844000	0.094684000
C	8.955004000	-1.542229000	0.036213000
H	9.590455000	-2.421736000	0.053195000
C	4.940692000	1.227435000	0.061144000
H	5.503781000	2.154737000	0.074537000
C	11.389757000	1.341849000	-0.071796000
S	-7.511013000	0.375773000	-0.087269000
S	-3.518260000	-1.551927000	0.019275000
C	-0.892096000	-0.618006000	0.034070000
C	-2.293968000	-0.289224000	-0.004028000
C	-4.825912000	-0.378421000	-0.054918000
C	-0.289314000	-1.860435000	0.115502000
C	-8.727855000	-0.891338000	-0.109058000
C	-2.897187000	0.952973000	-0.063978000
H	-2.334008000	1.880134000	-0.087273000
C	-10.152294000	-0.653942000	-0.181784000
H	-10.752984000	-1.557801000	-0.267132000
C	-6.203901000	-0.803358000	-0.069940000
C	-6.710836000	-2.089447000	-0.078503000
H	-6.084382000	-2.975554000	-0.074614000
C	-8.122609000	-2.134664000	-0.098541000
H	-8.694911000	-3.056743000	-0.112169000
C	-4.308673000	0.903535000	-0.093010000
H	-4.934785000	1.787691000	-0.145105000
C	-10.806093000	0.523360000	-0.173893000
H	1.746587000	-2.695665000	0.200001000
H	-0.853613000	-2.785426000	0.165768000
N	-10.162766000	1.776935000	-0.004714000
C	-10.075970000	2.197353000	1.399644000
C	-10.742207000	2.816555000	-0.850797000
H	-11.794711000	3.041172000	-0.593318000
H	-10.701380000	2.504222000	-1.898103000
H	-10.160745000	3.738003000	-0.743715000
H	-9.604054000	1.409594000	1.991086000
H	-9.455839000	3.097744000	1.467103000
H	-11.064980000	2.422522000	1.837145000
C	12.791304000	1.574552000	-0.097046000
N	13.937995000	1.783665000	-0.118169000
H	10.756070000	2.225654000	-0.084439000
H	-11.894399000	0.530883000	-0.300610000

Molecule Name : 2_b

S	-0.122308000	0.555418000	-0.256279000
S	7.702898000	0.790207000	-0.003178000
S	3.845986000	-1.378309000	0.059628000
C	1.175029000	-0.630110000	-0.186280000
C	2.554212000	-0.216655000	-0.197673000
C	5.081559000	-0.138056000	-0.110033000
C	0.647537000	-1.906495000	-0.120033000
C	8.998184000	-0.389388000	0.134173000
C	3.082124000	1.049433000	-0.387031000
H	2.465210000	1.922516000	-0.569940000
C	10.387258000	-0.048170000	0.191191000
H	11.083414000	-0.878703000	0.283833000
C	6.478439000	-0.467380000	-0.007789000
C	7.069045000	-1.718417000	0.100244000
H	6.497317000	-2.639814000	0.111219000
C	8.473966000	-1.671194000	0.179519000
H	9.104400000	-2.550306000	0.263660000
C	4.491213000	1.092050000	-0.337722000
H	5.064018000	2.002545000	-0.479355000
C	10.922228000	1.188109000	0.143267000
S	-7.945299000	0.415189000	-0.039718000
S	-3.986573000	-1.546494000	0.120137000
C	-1.355108000	-0.696262000	-0.222711000
C	-2.754117000	-0.355074000	-0.271445000
C	-5.284535000	-0.402653000	-0.191298000
C	-0.763947000	-1.944259000	-0.140033000
C	-9.183576000	-0.816940000	0.146023000
C	-3.346437000	0.850735000	-0.595951000
H	-2.775318000	1.727269000	-0.883758000
C	-10.603963000	-0.548323000	0.179305000
H	-11.227416000	-1.439847000	0.217390000
C	-6.665963000	-0.793034000	-0.049964000
C	-7.195216000	-2.061970000	0.091929000
H	-6.587628000	-2.961058000	0.099589000
C	-8.603601000	-2.071280000	0.203738000
H	-9.192505000	-2.976325000	0.313188000
C	-4.758523000	0.824473000	-0.551599000
H	-5.379883000	1.677696000	-0.801175000
C	-11.232505000	0.642809000	0.151888000

H	1.265372000	-2.797378000	-0.075837000
H	-1.337106000	-2.864790000	-0.116846000
N	-10.557205000	1.889589000	0.167770000
C	-10.304246000	2.400825000	1.521222000
C	-11.206603000	2.885547000	-0.679641000
H	-12.219372000	3.154957000	-0.324587000
H	-11.288123000	2.503465000	-1.701087000
H	-10.599207000	3.796161000	-0.700769000
H	-9.790210000	1.640131000	2.112670000
H	-9.657290000	3.282291000	1.456468000
H	-11.232709000	2.688147000	2.045941000
N	12.350128000	1.371123000	0.214140000
O	12.749810000	2.540176000	0.163401000
O	13.083219000	0.381133000	0.318953000
H	-12.327129000	0.666703000	0.115155000
H	10.389482000	2.124782000	0.052832000

Molecule Name: 2_c

S	-0.130402000	0.523911000	-0.335322000
S	7.689642000	0.756435000	-0.019797000
S	3.828420000	-1.392431000	0.096027000
C	1.162811000	-0.665055000	-0.255450000
C	2.544253000	-0.255945000	-0.285702000
C	5.071139000	-0.178262000	-0.174955000
C	0.631631000	-1.937439000	-0.159950000
C	8.983763000	-0.415804000	0.176439000
C	3.079110000	0.985318000	-0.580071000
H	2.467848000	1.838477000	-0.854019000
C	10.372815000	-0.060281000	0.258754000
H	11.060782000	-0.894593000	0.390831000
C	6.467236000	-0.503835000	-0.028311000
C	7.055903000	-1.748401000	0.125157000
H	6.486035000	-2.671148000	0.139191000
C	8.460944000	-1.695393000	0.239740000
H	9.090478000	-2.571020000	0.359769000
C	4.489400000	1.027883000	-0.517829000
H	5.069021000	1.917815000	-0.739335000
C	10.915808000	1.175351000	0.193080000

S	-7.948430000	0.431191000	-0.019934000
S	-4.000305000	-1.548106000	0.124760000
C	-1.368104000	-0.722373000	-0.271145000
C	-2.766518000	-0.375698000	-0.316460000
C	-5.296421000	-0.407442000	-0.206996000
C	-0.781090000	-1.969972000	-0.168398000
C	-9.192433000	-0.789620000	0.201215000
C	-3.356390000	0.822828000	-0.669974000
H	-2.783924000	1.686974000	-0.990588000
C	-10.609984000	-0.509819000	0.259529000
H	-11.238955000	-1.396088000	0.323208000
C	-6.678291000	-0.786562000	-0.038208000
C	-7.213934000	-2.049674000	0.127835000
H	-6.612558000	-2.952904000	0.135013000
C	-8.620572000	-2.047149000	0.263739000
H	-9.213890000	-2.946598000	0.393960000
C	-4.768533000	0.805270000	-0.609076000
H	-5.388559000	1.653718000	-0.877744000
C	-11.230086000	0.685410000	0.230222000
H	1.247276000	-2.829339000	-0.107984000
H	-1.357386000	-2.887917000	-0.125027000
N	-10.543442000	1.926788000	0.212975000
C	-10.275092000	2.462510000	1.553713000
C	-11.194702000	2.910154000	-0.647439000
H	-12.202508000	3.192948000	-0.288313000
H	-11.288471000	2.508587000	-1.660350000
H	-10.581943000	3.816371000	-0.692086000
H	-9.758104000	1.710691000	2.153986000
H	-9.625191000	3.339859000	1.465874000
H	-11.196919000	2.763736000	2.082632000
C	12.371217000	1.342295000	0.300210000
O	12.731859000	2.652526000	0.213074000
O	13.191531000	0.454097000	0.448680000
H	13.703484000	2.662491000	0.294035000
H	-12.325171000	0.718295000	0.220093000
H	10.319554000	2.073378000	0.062232000

Molecule name: 2

S	0.000000000	0.608687000	-0.000046000
S	7.818743000	0.633057000	0.000010000
S	3.918621000	-1.449654000	-0.000151000
C	1.263902000	-0.611061000	-0.000072000

C	2.653459000	-0.233422000	-0.000103000
C	5.180365000	-0.225549000	-0.000142000
C	0.705268000	-1.877257000	-0.000023000
C	9.088758000	-0.585497000	-0.000005000
C	3.208796000	1.035769000	-0.000159000
H	2.611496000	1.941082000	-0.000149000
C	10.489860000	-0.338593000	0.000049000
H	11.097638000	-1.240845000	0.000049000
C	6.570443000	-0.593936000	-0.000101000
C	7.126412000	-1.869475000	-0.000140000
H	6.530288000	-2.775240000	-0.000205000
C	8.527579000	-1.860984000	-0.000085000
H	9.137542000	-2.758475000	-0.000099000
C	4.617866000	1.039685000	-0.000112000
H	5.210215000	1.948598000	-0.000127000
C	11.189167000	0.844776000	0.000103000
N	13.783238000	0.793107000	0.000277000
C	12.619303000	0.821529000	0.000193000
C	10.567737000	2.130693000	0.000127000
N	10.059856000	3.179079000	0.000068000
S	-7.818743000	0.633058000	-0.000031000
S	-3.918621000	-1.449653000	0.000099000
C	-1.263902000	-0.611061000	-0.000013000
C	-2.653459000	-0.233422000	-0.000001000
C	-5.180365000	-0.225549000	0.000071000
C	-0.705269000	-1.877257000	-0.000031000
C	-9.088758000	-0.585497000	0.000084000
C	-3.208796000	1.035770000	-0.000016000
H	-2.611496000	1.941083000	-0.000080000
C	-10.489859000	-0.338593000	0.000083000
H	-11.097637000	-1.240845000	0.000137000
C	-6.570443000	-0.593936000	0.000086000
C	-7.126411000	-1.869474000	0.000179000
H	-6.530288000	-2.775239000	0.000248000
C	-8.527579000	-1.860984000	0.000174000
H	-9.137542000	-2.758475000	0.000239000
C	-4.617866000	1.039685000	-0.000045000
H	-5.210215000	1.948599000	-0.000071000
C	-11.189167000	0.844775000	0.000021000
N	-13.783238000	0.793106000	-0.000039000
C	-12.619304000	0.821528000	-0.000006000
C	-10.567738000	2.130693000	-0.000069000
N	-10.059856000	3.179078000	-0.000063000

H	1.300054000	-2.784442000	-0.000056000
H	-1.300055000	-2.784441000	0.000014000

Molecule name: 3_a

S	0.199639000	-0.108925000	-0.055619000
C	-2.431623000	0.881401000	-0.020319000
C	1.507758000	1.077419000	0.026110000
C	2.893721000	0.793520000	0.035061000
H	3.525391000	1.678563000	0.079091000
C	-1.023908000	1.146570000	-0.003412000
C	-0.426421000	2.407416000	0.058883000
H	-1.007491000	3.322491000	0.096080000
C	0.970966000	2.364732000	0.076958000
H	1.603134000	3.245820000	0.128617000
C	-2.983279000	-0.369161000	-0.006890000
C	3.570255000	-0.408708000	-0.002288000
N	6.163879000	-0.407464000	0.034024000
C	4.998953000	-0.413966000	0.017436000
C	2.924427000	-1.679671000	-0.059150000
N	2.399661000	-2.719526000	-0.104883000
H	-3.068330000	1.760999000	-0.032943000
N	-4.302805000	-0.684132000	-0.094271000
C	-4.760763000	-2.020552000	0.257481000
C	-5.304646000	0.365468000	-0.168088000
H	-5.417996000	0.898239000	0.788080000
H	-5.029626000	1.091157000	-0.940199000
H	-6.267110000	-0.076107000	-0.437312000
H	-5.564389000	-2.331124000	-0.418836000
H	-3.934525000	-2.728834000	0.159649000
H	-5.137695000	-2.068517000	1.289842000
H	-2.333375000	-1.238838000	0.063054000

Molecule name: 3_b

S	-0.158518000	-0.989035000	-0.126946000
C	-2.385770000	0.736988000	-0.028605000
C	1.456443000	-0.250500000	-0.037765000

C	2.561021000	-1.156169000	-0.074953000
H	2.253223000	-2.199466000	-0.149179000
C	-0.960016000	0.560023000	-0.028196000
C	-0.008607000	1.574678000	0.053358000
H	-0.290430000	2.620497000	0.120092000
C	1.322811000	1.131604000	0.051047000
H	2.183018000	1.780105000	0.113573000
C	-3.297465000	-0.276197000	-0.022845000
C	3.919465000	-1.067112000	-0.043641000
H	-2.717546000	1.771149000	-0.023020000
N	-4.656124000	-0.163984000	-0.106223000
C	-5.494320000	-1.274714000	0.318876000
C	-5.273508000	1.149688000	-0.143076000
H	-5.202125000	1.673022000	0.823265000
H	-4.790752000	1.766568000	-0.907632000
H	-6.329527000	1.042306000	-0.403664000
H	-6.408644000	-1.302836000	-0.283320000
H	-4.957414000	-2.215763000	0.172486000
H	-5.780225000	-1.202068000	1.379725000
N	4.735307000	0.098537000	0.048920000
O	4.215477000	1.223078000	0.117761000
O	5.960089000	-0.092562000	0.055574000
H	4.529476000	-1.957928000	-0.092013000
H	-2.951879000	-1.306770000	0.030072000

Molecule Name: 3_c

S	0.420678000	0.033527000	-0.058766000
C	-2.284418000	0.823961000	-0.049755000
C	1.635311000	1.311659000	0.055056000
C	3.061899000	1.188404000	0.085776000
H	3.531870000	2.170372000	0.154797000
C	-0.892217000	1.194295000	-0.011966000
C	-0.399939000	2.492211000	0.069538000
H	-1.046139000	3.363267000	0.106894000
C	1.001564000	2.549703000	0.109248000
H	1.565503000	3.475277000	0.178519000
C	-2.749467000	-0.454742000	-0.019580000
C	3.946639000	0.153169000	0.049356000
H	-2.981088000	1.656643000	-0.096191000
N	-4.051201000	-0.866234000	-0.143819000
C	-4.427729000	-2.174769000	0.367791000
C	-5.108638000	0.121138000	-0.249204000

H	-5.273050000	0.666985000	0.694118000
H	-4.860587000	0.847997000	-1.029222000
H	-6.040338000	-0.378718000	-0.527895000
H	-5.268931000	-2.571465000	-0.210758000
H	-3.584971000	-2.863991000	0.265141000
H	-4.721222000	-2.145905000	1.429490000
C	3.634242000	-1.264877000	-0.041882000
O	2.529965000	-1.786762000	-0.103416000
O	4.768557000	-2.025723000	-0.054600000
H	4.457382000	-2.947098000	-0.118536000
H	5.004033000	0.391335000	0.091568000
H	-2.046554000	-1.278522000	0.086930000

Molecule name:3

S	0.000015000	0.072378000	-0.000074000
C	2.664278000	-0.919271000	-0.000095000
C	-1.251155000	-1.153874000	0.000044000
C	-2.664243000	-0.919221000	-0.000013000
H	-3.262321000	-1.827486000	-0.000040000
C	1.251196000	-1.153907000	0.000008000
C	0.699420000	-2.434179000	0.000162000
H	1.309757000	-3.330742000	0.000250000
C	-0.699426000	-2.434167000	0.000195000
H	-1.309781000	-3.330714000	0.000322000
C	3.369524000	0.253858000	-0.000012000
C	-3.369504000	0.253907000	-0.000033000
N	-5.964133000	0.176116000	-0.000059000
C	-4.801288000	0.216005000	-0.000130000
C	-2.766395000	1.549950000	-0.000049000
N	-2.285652000	2.610160000	-0.000023000
H	3.262351000	-1.827527000	-0.000225000
C	2.766402000	1.549912000	0.000133000
C	4.801303000	0.215967000	-0.000139000
N	2.285499000	2.610048000	0.000378000
N	5.964157000	0.176325000	-0.000231000

Molecule Name: VCTO4ew

S	0.881734000	-0.989080000	-0.039382000
S	-6.822473000	-0.763100000	0.092998000
S	-2.929882000	1.252285000	-0.074166000
C	-0.319132000	0.293380000	-0.110263000
C	-1.724378000	-0.014791000	-0.186657000
C	-4.255501000	0.107581000	-0.271592000
C	0.302647000	1.527653000	-0.076739000
C	-8.152516000	0.375597000	-0.040021000
C	-2.338943000	-1.244578000	-0.355793000
H	-1.784892000	-2.170709000	-0.463405000
C	-9.518859000	0.014883000	0.110796000
H	-10.220786000	0.839521000	0.037128000
C	-5.647049000	0.488570000	-0.233318000
C	-6.258662000	1.731466000	-0.416426000
C	-7.673445000	1.667488000	-0.302548000
C	-3.744666000	-1.175240000	-0.401332000
H	-4.376663000	-2.044944000	-0.545814000
C	-10.108968000	-1.209290000	0.334549000
N	-12.692675000	-1.336042000	0.542299000
C	-11.532809000	-1.285721000	0.450078000
C	-9.397602000	-2.440787000	0.460385000
N	-8.830957000	-3.453490000	0.564826000
S	8.559665000	-1.412685000	-0.486608000
S	4.903465000	0.852343000	-0.014072000
C	2.204051000	0.164838000	0.038825000
C	3.572164000	-0.284366000	0.118733000
C	6.101748000	-0.412380000	0.227019000
C	1.710657000	1.456584000	0.006980000
C	10.003767000	-0.465551000	-0.202268000
C	4.059270000	-1.563348000	0.310910000

H	3.414449000	-2.427253000	0.434066000
C	11.318721000	-0.977936000	-0.547515000
H	12.138177000	-0.279875000	-0.390746000
C	7.528934000	-0.158220000	0.181899000
C	8.276940000	0.936020000	0.582406000
C	9.684244000	0.760263000	0.357088000
C	5.469263000	-1.634157000	0.368760000
H	6.016292000	-2.555331000	0.536563000
C	11.611645000	-2.196580000	-1.027906000
H	2.350068000	2.331727000	0.049767000
H	-0.244502000	2.463770000	-0.115852000
C	10.683160000	1.825009000	0.729001000
H	10.717145000	1.979327000	1.815586000
H	11.696075000	1.578038000	0.404576000
H	10.418787000	2.789158000	0.277821000
C	7.722450000	2.180355000	1.225430000
H	7.631934000	3.006015000	0.506228000
H	6.733142000	2.011068000	1.656785000
H	8.379502000	2.529011000	2.029756000
C	-5.519169000	3.007764000	-0.726500000
H	-5.057515000	3.442107000	0.170037000
H	-4.720019000	2.843011000	-1.456015000
H	-6.191298000	3.762580000	-1.141982000
C	-8.542418000	2.886143000	-0.470250000
H	-8.467385000	3.286243000	-1.489171000
H	-9.597915000	2.687403000	-0.278212000
H	-8.231158000	3.684047000	0.213760000
H	12.635376000	-2.473439000	-1.257595000
H	10.853180000	-2.954858000	-1.205844000

Molecule Name: VCTO4a

S	0.771058000	-0.600880000	-0.288473000
S	8.484953000	-0.951371000	-0.165840000
S	4.733486000	1.314142000	0.200641000
C	2.066378000	0.570140000	-0.066660000
C	3.439994000	0.147720000	0.000757000

C	5.968109000	0.053945000	0.204682000
C	1.539474000	1.846015000	0.020114000
C	9.881538000	0.043128000	0.215665000
C	3.961220000	-1.135547000	-0.059981000
H	3.341574000	-2.018505000	-0.172451000
C	11.224415000	-0.396616000	0.075800000
H	11.977420000	0.345605000	0.321537000
C	7.381077000	0.323084000	0.298200000
C	8.067915000	1.469510000	0.710433000
C	9.477988000	1.311368000	0.660623000
C	5.362823000	-1.185368000	0.052133000
H	5.925289000	-2.112847000	0.036163000
C	11.740335000	-1.611588000	-0.320884000
N	14.316785000	-1.906959000	-0.414932000
C	13.159568000	-1.780772000	-0.374914000
C	10.954670000	-2.745115000	-0.688960000
N	10.328187000	-3.679758000	-0.991975000
S	-6.945308000	-0.548733000	-0.230539000
S	-3.097662000	1.530355000	-0.122981000
C	-0.457350000	0.656380000	-0.274464000
C	-1.850896000	0.328463000	-0.424291000
C	-4.388134000	0.411094000	-0.556008000
C	0.133833000	1.895603000	-0.095123000
C	-8.306579000	0.561592000	-0.219537000
C	-2.431836000	-0.865860000	-0.809106000
H	-1.851009000	-1.746521000	-1.063900000
C	-9.678006000	0.109952000	-0.162722000
H	-10.403684000	0.794305000	-0.589614000
C	-5.787793000	0.756698000	-0.480063000
C	-6.442406000	1.978146000	-0.549003000
C	-7.860409000	1.866756000	-0.392563000
C	-3.839929000	-0.820400000	-0.882501000
H	-4.448707000	-1.661886000	-1.194267000
C	-10.160418000	-1.087572000	0.301336000
H	-0.436123000	2.817777000	-0.062304000
H	2.155092000	2.728848000	0.158715000
C	-8.778166000	3.062841000	-0.417274000

H	-8.928656000	3.450513000	-1.434970000
H	-9.762557000	2.818737000	-0.009479000
H	-8.374988000	3.887857000	0.181779000
C	-5.767534000	3.305835000	-0.781499000
H	-5.503497000	3.803845000	0.161962000
H	-4.846612000	3.198839000	-1.361086000
H	-6.425763000	3.986760000	-1.330418000
C	7.400920000	2.736483000	1.181979000
H	6.974386000	3.309824000	0.348565000
H	6.585406000	2.526063000	1.881686000
H	8.111073000	3.390251000	1.693896000
C	10.420012000	2.413801000	1.067967000
H	10.299602000	2.662337000	2.129766000
H	11.469057000	2.156793000	0.913579000
H	10.221093000	3.328324000	0.497324000
N	-9.458774000	-1.914846000	1.174593000
N	-11.402859000	-1.587288000	-0.103630000
C	-8.799539000	-1.403981000	2.363465000
H	-9.204530000	-1.900194000	3.259380000
H	-7.715418000	-1.576286000	2.337641000
H	-8.974539000	-0.330606000	2.446518000
C	-9.434405000	-3.359040000	1.017200000
H	-8.395707000	-3.717232000	0.980654000
H	-9.935954000	-3.873266000	1.852131000
H	-9.935063000	-3.635110000	0.088291000
C	-12.025852000	-1.064757000	-1.307195000
H	-12.760397000	-1.792182000	-1.672550000
H	-12.555160000	-0.110757000	-1.141133000
H	-11.266275000	-0.910215000	-2.076620000
C	-12.358982000	-2.011759000	0.915199000
H	-13.022669000	-1.184509000	1.217222000
H	-12.983098000	-2.827052000	0.531021000
H	-11.829593000	-2.364819000	1.800801000

Molecule Name : VCTO4b

S	0.083483000	-0.315566000	-0.653293000

S	7.737036000	-0.749432000	-0.002418000
S	3.993107000	1.525576000	0.257130000
C	1.353347000	0.849132000	-0.295269000
C	2.739486000	0.472516000	-0.366921000
C	5.271198000	0.404963000	-0.216101000
C	0.795000000	2.069541000	0.040353000
C	9.136701000	0.254493000	0.346957000
C	3.302392000	-0.680491000	-0.894317000
H	2.712219000	-1.465993000	-1.353392000
C	10.482929000	-0.180156000	0.408981000
H	11.189385000	0.589823000	0.700646000
C	6.669696000	0.630862000	0.044885000
C	7.357447000	1.810450000	0.359777000
C	8.745614000	1.596726000	0.534342000
C	4.705394000	-0.716254000	-0.808668000
H	5.301820000	-1.536334000	-1.193808000
C	11.149150000	-1.340709000	0.142910000
S	-7.609450000	-0.570530000	-0.227264000
S	-3.835309000	1.614525000	0.027058000
C	-1.178289000	0.874277000	-0.368864000
C	-2.566573000	0.525221000	-0.515240000
C	-5.108267000	0.531023000	-0.530529000
C	-0.615248000	2.084865000	0.000665000
C	-9.007598000	0.469698000	-0.004172000
C	-3.127109000	-0.612792000	-1.066111000
H	-2.531426000	-1.418275000	-1.483527000
C	-10.357691000	-0.040888000	0.047249000
H	-11.128512000	0.673401000	-0.221894000
C	-6.513166000	0.804837000	-0.343094000
C	-7.212816000	1.995484000	-0.210034000
C	-8.616486000	1.804207000	-0.009857000
C	-4.537402000	-0.610192000	-1.074601000
H	-5.133390000	-1.412466000	-1.495238000
C	-10.772012000	-1.317623000	0.331485000
H	-1.209605000	2.965888000	0.217079000
H	1.392604000	2.940342000	0.289610000
C	-9.575465000	2.953895000	0.170053000

H	-9.800358000	3.459535000	-0.779919000
H	-10.524606000	2.620037000	0.597477000
H	-9.165280000	3.713325000	0.846000000
C	-6.599499000	3.370334000	-0.284215000
H	-6.342207000	3.759579000	0.710842000
H	-5.684814000	3.377533000	-0.882848000
H	-7.296229000	4.083330000	-0.736848000
C	6.712127000	3.167507000	0.477260000
H	5.995499000	3.342991000	-0.331421000
H	6.168916000	3.282766000	1.424408000
H	7.457298000	3.965186000	0.432429000
C	9.684440000	2.729212000	0.859329000
H	9.343734000	3.269481000	1.749792000
H	10.706841000	2.401627000	1.050985000
H	9.724731000	3.453975000	0.036594000
N	-9.985819000	-2.244923000	1.012254000
N	-12.018210000	-1.797293000	-0.083551000
C	-9.303349000	-1.914789000	2.251292000
H	-9.681776000	-2.544804000	3.072073000
H	-8.219749000	-2.071105000	2.172572000
H	-9.481869000	-0.868004000	2.499598000
C	-9.928744000	-3.642723000	0.620117000
H	-8.882245000	-3.955236000	0.496586000
H	-10.387749000	-4.304279000	1.371902000
H	-10.451353000	-3.779176000	-0.327439000
C	-12.733570000	-1.108725000	-1.143806000
H	-13.462350000	-1.797599000	-1.586936000
H	-13.285467000	-0.222110000	-0.787436000
H	-12.029536000	-0.791641000	-1.916234000
C	-12.892312000	-2.435625000	0.896612000
H	-13.568414000	-1.705472000	1.371627000
H	-13.505599000	-3.203890000	0.411458000
H	-12.296110000	-2.906987000	1.678470000
N	10.563996000	-2.562910000	-0.364824000
O	9.457232000	-2.876936000	0.093162000
O	11.164470000	-3.181074000	-1.235140000
N	12.590659000	-1.386748000	0.368423000

O	13.118689000	-2.489643000	0.475771000
O	13.180032000	-0.306737000	0.493515000

Molecule Name: VCTO4c

S	0.077578000	-0.597987000	-0.012225000
S	7.765066000	-0.745096000	0.022786000
S	4.005763000	1.418091000	0.254800000
C	1.342370000	0.613135000	0.159343000
C	2.722186000	0.223589000	0.306097000
C	5.249461000	0.199741000	0.523064000
C	0.791560000	1.879782000	0.121034000
C	9.160501000	0.281211000	0.325758000
C	3.255800000	-1.038047000	0.503338000
H	2.643285000	-1.929646000	0.584117000
C	10.535033000	-0.049034000	0.121336000
H	11.185839000	0.756438000	0.438453000
C	6.664854000	0.504699000	0.541577000
C	7.335003000	1.665524000	0.926587000
C	8.743497000	1.539747000	0.798951000
C	4.661946000	-1.050063000	0.620051000
H	5.238932000	-1.951517000	0.795501000
C	11.243468000	-1.109528000	-0.392279000
S	-7.653017000	-0.619394000	-0.185337000
S	-3.826941000	1.477481000	-0.273578000
C	-1.175113000	0.630312000	-0.132186000
C	-2.558181000	0.261156000	-0.296759000
C	-5.083831000	0.282451000	-0.586804000
C	-0.612008000	1.890471000	-0.041954000
C	-9.018113000	0.444628000	-0.489662000
C	-3.109543000	-0.988551000	-0.507294000
H	-2.511436000	-1.891814000	-0.572195000
C	-10.389264000	-0.011279000	-0.412117000
H	-11.082054000	0.505777000	-1.068321000
C	-6.488618000	0.617326000	-0.654604000
C	-7.142987000	1.781707000	-1.026190000
C	-8.568142000	1.684247000	-0.924217000

C	-4.512436000	-0.976804000	-0.668346000
H	-5.098060000	-1.867427000	-0.868062000
C	-10.900005000	-1.046308000	0.328584000
H	-1.198947000	2.801069000	-0.096261000
H	1.386207000	2.782518000	0.215292000
C	-9.488125000	2.829070000	-1.264542000
H	-9.579118000	2.980478000	-2.349697000
H	-10.493770000	2.661788000	-0.869793000
H	-9.124850000	3.773172000	-0.841212000
C	-6.466282000	3.036546000	-1.515200000
H	-6.324992000	3.768446000	-0.707594000
H	-5.482274000	2.829903000	-1.943549000
H	-7.067972000	3.525898000	-2.288486000
C	6.673431000	2.910224000	1.461084000
H	6.452930000	3.634137000	0.664604000
H	5.729391000	2.680563000	1.961696000
H	7.315930000	3.416786000	2.187707000
C	9.655114000	2.684411000	1.162521000
H	9.653460000	2.859518000	2.246539000
H	10.691073000	2.529175000	0.858924000
H	9.315349000	3.612451000	0.688862000
N	-10.284592000	-1.572869000	1.460499000
N	-12.099834000	-1.678493000	-0.020776000
C	-9.666817000	-0.732937000	2.470106000
H	-10.075170000	-0.984027000	3.460949000
H	-8.576491000	-0.860903000	2.507348000
H	-9.882335000	0.314642000	2.255273000
C	-10.205801000	-3.003675000	1.701199000
H	-9.155512000	-3.321267000	1.779340000
H	-10.711542000	-3.286875000	2.637025000
H	-10.675372000	-3.539762000	0.875492000
C	-12.615298000	-1.532949000	-1.370625000
H	-13.309216000	-2.356312000	-1.577922000
H	-13.163595000	-0.587605000	-1.525060000
H	-11.790381000	-1.575294000	-2.085133000
C	-13.140971000	-1.829441000	0.991750000
H	-13.835683000	-0.972835000	0.989769000

H	-13.722001000	-2.739786000	0.802747000
H	-12.689758000	-1.901642000	1.981932000
C	10.610399000	-2.330618000	-0.927751000
O	9.471708000	-2.690657000	-0.669660000
O	11.379610000	-3.024681000	-1.792073000
H	10.833478000	-3.786105000	-2.063837000
C	12.727971000	-1.034209000	-0.366503000
O	13.496051000	-1.969189000	-0.454606000
O	13.196403000	0.240895000	-0.188575000
H	14.163937000	0.139924000	-0.128390000

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S	1.646087000	-0.845966000	-0.478041000
S	9.345355000	-1.345065000	-0.691609000
S	5.697164000	0.827854000	0.162799000
C	2.988620000	0.226072000	-0.097691000
C	4.344003000	-0.267364000	-0.069720000
C	6.864902000	-0.489392000	0.127774000
C	2.519226000	1.502560000	0.142696000
C	10.785870000	-0.543254000	-0.101945000
C	4.803447000	-1.565076000	-0.190391000
H	4.141194000	-2.413071000	-0.329811000
C	12.110273000	-0.991743000	-0.495026000
H	12.929644000	-0.375850000	-0.130173000
C	8.296155000	-0.272112000	0.220793000
C	9.037005000	0.664020000	0.922221000
C	10.452265000	0.510931000	0.731416000
C	6.207982000	-1.686950000	-0.082454000
H	6.731897000	-2.635298000	-0.133005000
C	12.413880000	-2.063500000	-1.244409000
S	-6.053761000	-0.450126000	-0.301022000
S	-2.130408000	1.414548000	-0.056686000
C	0.472946000	0.454236000	-0.311746000
C	-0.934407000	0.208919000	-0.508407000
C	-3.464243000	0.420457000	-0.638477000
C	1.115901000	1.630613000	0.023300000

C	-7.368386000	0.711592000	-0.198899000
C	-1.562627000	-0.898089000	-1.045402000
H	-1.018166000	-1.763432000	-1.409394000
C	-8.757130000	0.309976000	-0.127362000
H	-9.461774000	1.021511000	-0.545674000
C	-4.849929000	0.818270000	-0.515034000
C	-5.454236000	2.065028000	-0.510023000
C	-6.873454000	2.002570000	-0.323284000
C	-2.969336000	-0.780360000	-1.117209000
H	-3.612639000	-1.546594000	-1.535905000
C	-9.277947000	-0.867163000	0.343989000
H	0.587659000	2.566779000	0.169480000
H	3.172108000	2.329569000	0.401745000
C	-7.739897000	3.235165000	-0.271650000
H	-7.896854000	3.674676000	-1.267206000
H	-8.724213000	3.012966000	0.149083000
H	-7.287479000	4.015288000	0.352207000
C	-4.735346000	3.376024000	-0.700949000
H	-4.520652000	3.870321000	0.256907000
H	-3.783451000	3.247351000	-1.222033000
H	-5.344685000	4.070926000	-1.289107000
C	8.463779000	1.721350000	1.829516000
H	8.413570000	2.701494000	1.335461000
H	7.453560000	1.469376000	2.160227000
H	9.084554000	1.846329000	2.723540000
C	11.444709000	1.418789000	1.410216000
H	11.409314000	1.305621000	2.501809000
H	12.471883000	1.221127000	1.096853000
H	11.230615000	2.472298000	1.191838000
N	-8.606310000	-1.722062000	1.214261000
N	-10.546302000	-1.319107000	-0.043351000
C	-7.869615000	-1.235929000	2.366499000
H	-8.236270000	-1.731683000	3.278731000
H	-6.791904000	-1.430359000	2.281423000
H	-8.016405000	-0.159774000	2.467333000
C	-8.616566000	-3.164119000	1.039425000
H	-7.589197000	-3.544102000	0.939711000

H	-9.080602000	-3.676082000	1.896781000
H	-9.175320000	-3.419334000	0.138098000
C	-11.164342000	-0.771332000	-1.237621000
H	-11.935072000	-1.466716000	-1.591044000
H	-11.649876000	0.204899000	-1.065647000
H	-10.410483000	-0.649804000	-2.018581000
C	-11.504093000	-1.698556000	0.991053000
H	-12.126835000	-0.842868000	1.302036000
H	-12.169433000	-2.486518000	0.618802000
H	-10.975495000	-2.072879000	1.868447000
H	11.656441000	-2.734908000	-1.641076000
H	13.445205000	-2.302788000	-1.482464000