Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Supporting Information

Unravelling the Impact of Sulfur atom Oxidation and Donor-Acceptor Effects on the Performance of Blue TADF Emitters: A Detailed Computational Study

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CONTENT CAPTIONS

Table S1. Calculated the HOMO, LUMO energies, and E_g gap of reference molecules along with experimental values using 6-31+G* level of theory. (All energies are in eV)

Molecules	BP86	O3LYP	B3LYP	PBE0	M06	BMK	M06-2X	CAM-B3LYP	WB97XD	M06-HF	Exp.
HOMO											
PXZ-Ph-SO_2	-4.60	-4.81	-5.25	-5.45	-5.59	-5.92	-6.62	-6.61	-7.19	-8.43	-5.59
PTZ-Ph-SO_2	-4.81	-5.06	-5.48	-5.67	-5.72	-6.20	-6.74	-6.83	-7.34	-8.42	-6.11
DMAC-Ph-SO_2	-4.90	-5.13	-5.53	-5.75	-5.84	-5.13	-6.81	-6.87	-7.41	-8.41	-5.92
DPA-Ph-SO_2	-4.88	-5.13	-5.49	-5.66	-5.77	-6.11	-6.65	-6.76	-7.27	-8.21	-5.89
LUMO											
PXZ-Ph-SO_2	-2.96	-2.43	-2.24	-2.10	-2.06	-1.46	-1.36	-1.02	-0.43	-0.46	-2.79
PTZ-Ph-SO_2	-2.98	-2.37	-2.20	-2.08	-2.03	-1.44	-1.35	-0.99	-0.43	-0.46	-3.34
DMAC-Ph-SO_2	-2.87	-2.28	-2.10	-1.96	-1.93	-2.28	-1.23	-0.88	-0.30	-0.33	-2.92
DPA-Ph-SO_2	-2.30	-1.72	-1.56	-1.42	-1.40	-0.85	-0.78	-0.38	-0.21	-0.23	-2.62
E_g											
PXZ-Ph-SO_2	1.63	2.38	3.01	3.35	3.53	4.46	5.26	5.59	6.76	7.97	2.80
PTZ-Ph-SO_2	1.83	2.69	3.28	3.59	3.69	4.77	5.39	5.84	6.92	7.97	2.77
DMAC-Ph-SO_2	2.02	2.85	3.44	3.78	3.91	2.85	5.58	5.99	7.11	8.08	3.00
DPA-Ph-SO_2	2.57	3.42	3.94	4.24	4.37	5.26	5.87	6.38	7.48	7.99	3.27

Table S2. Calculated the HOMO, LUMO energies, and E_g gap of reference molecules using B3LYP functional along with different basis sets. (All energies are in eV)

Molecules	6-31G*	6-31G**	6-31+G*	6-31+G**	6-311G*	6-311G**	6-311+G**
HOMO							
PXZ-Ph-SO_2	-4.90	-4.91	-5.25	-5.26	-5.16	-5.17	-5.33
PTZ-Ph-SO_2	-5.21	-5.21	-5.48	-5.48	-5.45	-5.45	-5.53
DMAC-Ph-SO_2	-5.25	-5.22	-5.53	-5.54	-5.51	-5.51	-5.60
DPA-Ph-SO_2	-5.21	-5.22	-5.49	-5.50	-5.46	-5.47	-5.56
LUMO							

PXZ-Ph-SO_2	-1.88	-1.89	-2.10	-2.25	-2.17	-2.18	-2.30
PTZ-Ph-SO_2	-1.86	-1.87	-2.08	-2.21	-2.13	-2.14	-2.25
DMAC-Ph-SO_2	-1.75	-1.17	-1.96	-2.10	-2.03	-2.03	-2.15
DPA-Ph-SO_2	-1.16	-1.17	-1.56	-1.56	-1.44	-1.45	1.61
E_g							
PXZ-Ph-SO_2	3.02	3.02	3.01	3.01	2.99	2.99	3.03
PTZ-Ph-SO_2	3.35	3.35	3.28	3.27	3.32	3.31	3.28
DMAC-Ph-SO_2	3.50	4.04	3.44	3.44	3.48	3.48	3.45
DPA-Ph-SO_2	4.05	4.05	3.93	3.94	4.01	4.02	3.95

Table S3. Calculated the vertical singlet (S_1) and triplet (T_1) energies, singlet-triplet energy differences (ΔE_{ST}) of reference molecules along with experimental values using a 6-31+G* basis set. (All energies are in eV)

Molecules	BP86	O3LYP	B3LYP	PBE0	M06	BMK	M06-2X	CAM-B3LYP	WB97XD	M06-HF	Exp.
	Singlet (S_1)										
PXZ-Ph-SO_2	1.67	2.19	2.50	2.68	**2.74**	3.19	3.40	3.51	3.67	4.11	**2.73**
PTZ-Ph-SO_2	1.94	2.47	2.79	2.97	**3.00**	3.50	3.69	3.81	3.93	4.16	**3.02**
DMAC-Ph-SO_2	2.08	2.57	2.87	3.04	**3.10**	3.53	3.72	3.83	3.98	4.36	**3.00**
DPA-Ph-SO_2	2.72	3.12	3.42	3.45	**3.44**	3.76	3.94	3.99	3.97	4.23	**3.30**
	Triplet (T_1)										
PXZ-Ph-SO_2	1.66	2.18	2.49	2.66	**2.74**	3.11	3.27	2.84	2.99	3.59	**2.65**
PTZ-Ph-SO_2	1.93	2.46	2.76	2.88	**2.89**	3.25	3.40	3.01	3.15	3.69	**2.61**
DMAC-Ph-SO_2	2.07	2.56	2.86	3.02	**3.09**	3.52	3.71	3.25	3.41	4.09	**2.91**
DPA-Ph-SO_2	2.47	2.72	2.83	2.78	**2.82**	3.09	3.26	2.91	3.04	3.54	**2.76**
	Energy Gap (ΔE_{ST})										
PXZ-Ph-SO_2	0.01	0.01	0.01	0.02	**0.01**	0.08	0.13	0.67	0.68	0.52	**0.08**
PTZ-Ph-SO_2	0.01	0.01	0.02	0.09	**0.11**	0.25	0.28	0.80	0.78	0.47	**0.41**
DMAC-Ph-SO_2	0.01	0.01	0.01	0.02	**0.01**	0.02	0.01	0.59	0.57	0.27	**0.09**
DPA-Ph-SO_2	0.26	0.40	0.59	0.67	**0.63**	0.67	0.68	1.08	0.93	0.69	**0.54**

Table S4. Calculated bond Lengths (Å), bond angle (˚), and dihedral Angles (˚), between the donor and the acceptor at optimized S_0 states at B3LYP/6-31+G* level of theory.

Molecules	d_1	d_1'	d_2	d_3	d_4	d_5	θ	δ	δ'
PXZ-Ph-SO	1.52		1.84	1.83	1.43	1.43	97.78	85.63	98.43
PXZ-3Py-SO	1.52		1.83	1.82	1.41	1.40	98.64	32.37	29.87
PXZ-2Py-SO	1.52		1.84	1.85	1.43	1.43	95.53	-97.11	84.71
PXZ-Ph-SO_2	1.47	1.47	1.81	1.81	1.43	1.43	104.83	-86.28	93.02
PXZ-3Py-SO_2	1.48	1.47	1.79	1.79	1.40	1.40	105.76	27.67	27.64
PXZ-2Py-SO_2	1.47	1.47	1.83	1.83	1.43	1.43	102.97	-97.57	82.69
PTZ-Ph-SO	1.52		1.84	1.84	1.44	1.44	98.05	-97.10	97.09
PTZ-3Py-SO	1.52		1.83	1.84	1.43	1.43	97.71	-20.20	20.25
PTZ-2Py-SO	1.52		1.85	1.85	1.43	1.43	96.91	-83.29	83.27
PTZ-Ph-SO_2	1.47	1.47	1.81	1.81	1.44	1.44	104.99	-82.47	82.46
PTZ-3Py-SO_2	1.79	1.79	1.79	1.79	1.40	1.40	105.81	-17.49	17.49
PTZ-2Py-SO_2	1.47	1.48	1.83	1.83	1.43	1.43	104.37	-97.75	96.06
DMAC-Ph-SO	1.52		1.84	1.83	1.44	1.44	97.84	81.43	100.09
DMAC-3Py-SO	1.52		1.83	1.84	1.43	1.43	97.75	-93.17	86.89
DMAC-2Py-SO	1.52		1.84	1.85	1.43	1.43	95.90	-79.79	101.12
DMAC-Ph-SO_2	1.47	1.47	1.81	1.81	1.43	1.43	104.98	-80.96	80.96
DMAC-3Py-SO_2	1.47	1.47	1.80	1.80	1.43	1.43	105.00	-89.01	88.69
DMAC 2Py-SO_2	1.47	1.48	1.83	1.83	1.43	1.43	104.42	-81.51	80.77
DPA-Ph-SO	1.52		1.83	1.83	1.42	1.42	98.77	37.92	-37.32
DPA-3Py-SO	1.52		1.82	1.81	1.40	1.40	98.52	22.27	20.74
DPA-2Py-SO	1.52		1.83	1.84	1.41	1.41	96.79	-38.72	34.11
DPA-Ph-SO_2	1.48	1.48	1.80	1.80	1.41	1.41	105.65	-33.72	33.72
DPA-3Py-SO_2	1.48	1.47	1.79	1.79	1.39	1.39	105.91	18.94	19.23
DPA-2Py-SO_2	1.47	1.48	1.82	1.82	1.40	1.40	105.30	33.67	33.21

Table S5. The calculated HOMO and LUMO molecular orbital contribution (%) of PXZ, PTZ, DMAC, and DPA substituted molecules at M06/6-31+G* level of theory.

MOLECULES	ORBITAL	DONOR (CORE-I)	ACCEPTOR (CORE-II)	DONOR (CORE-III)
PXZ-Ph-SO	HOMO	88.58	-	8.14
	LUMO	-	94.40	2.42
PXZ-3Py-SO	HOMO	62.51	24.65	12.85
	LUMO	-	88.53	10.15
PXZ-2Py-SO	HOMO	-	-	96.31
	LUMO	-	94.77	0.19
PXZ-Ph-SO_2	HOMO	59.97	-	36.80
	LUMO	-	94.78	2.61
PXZ-3Py-SO_2	HOMO	44.71	25.07	30.23
	LUMO	10.37	78.47	11.16
PXZ-2Py-SO_2	HOMO	49.83	-	46.57
	LUMO	-	94.81	2.60
PTZ-Ph-SO	HOMO	48.76	-	48.63
	LUMO	3.90	92.20	3.90
PTZ-3Py-SO	HOMO	10.10	20.85	69.06
	LUMO	81.39	-	15.88
PTZ-2Py-SO	HOMO	48.88	-	48.84
	LUMO	46.27	-	46.31
PTZ-Ph-SO_2	HOMO	-	89.12	-
	LUMO	47.88	-	48.02
PTZ-3Py-SO_2	HOMO	28.51	42.97	28.51
	LUMO	46.77	-	46.52
PTZ-2Py-SO_2	HOMO	-	94.28	-
	LUMO	-	-	97.01
DMAC-Ph-SO	HOMO	95.76	-	-
	LUMO	-	94.17	-
DMAC-3Py-SO	HOMO	-	-	95.39
	LUMO	-	94.38	-

DMAC-2Py-SO	HOMO	95.33	-	-
	LUMO	-	95.50	-
DPA-Ph-SO	HOMO	43.743	-	27.22
	LUMO	10	78	-
DPA-3Py-SO	HOMO	-	34.00	62.00
	LUMO	22.76	73.12	-
DPA-2Py-SO	HOMO	-	26.49	70.65
	LUMO	38.42	60.77	-
DPA-Ph-SO_2	HOMO	46.81	31.38	21.81
	LUMO	12.92	77.75	-
DPA-3Py-SO_2	HOMO	-	-	96.51
	LUMO	-	95.29	-
DPA-2Py-SO_2	HOMO	36.29	29.43	34.28
	LUMO	-	80.02	10.19

Table S6. Calculated the vertical singlet (S_1) and triplet (T_1) energies, singlet-triplet energy differences (ΔE_{ST}) at B3LYP, PBE0, and M06/6-31+G* level of theory.

Molecules	**B3LYP**			**PBE0**			**M06**		
	S_1	**T_1**	**ΔE_{ST}**	**S_1**	**T_1**	**ΔE_{ST}**	**S_1**	**T_1**	**ΔE_{ST}**
PXZ-Ph-SO	2.84	2.80	0.04	3.01	2.76	0.25	3.05	2.78	0.27
PXZ-3Py-SO	3.62	3.10	0.52	3.76	3.08	0.68	3.73	3.10	0.63
PXZ-2Py-SO	2.51	2.48	0.03	2.68	2.63	0.05	2.72	2.68	0.04
PXZ-Ph-SO_2	2.50	2.49	0.01	2.61	2.59	0.02	2.75	2.74	0.01
PXZ-3Py-SO_2	3.47	2.98	0.49	3.68	3.00	0.67	3.62	3.05	0.57
PXZ-2Py-SO_2	2.43	2.41	0.02	2.60	2.56	0.04	2.65	2.62	0.03
PTZ-Ph-SO	3.15	2.96	0.19	3.32	2.93	0.39	3.20	2.94	0.20
PTZ-3Py-SO	3.79	3.15	0.64	3.67	3.07	0.60	3.84	3.24	0.60
PTZ-2Py-SO	2.97	2.94	0.02	3.15	2.95	0.21	3.17	2.94	0.23
PTZ-Ph-SO_2	2.79	2.76	0.02	2.97	2.88	0.09	3.00	2.89	0.11

PTZ-3Py-SO_2	3.67	3.13	0.55	3.82	3.11	0.71	3.79	3.15	0.64
PTZ-2Py-SO_2	2.68	2.66	0.02	2.87	2.83	0.04	2.89	2.86	0.03
DMAC-Ph-SO	3.22	3.20	0.02	3.38	3.24	0.14	3.41	3.23	0.18
DMAC-3Py-SO	2.67	2.65	0.03	2.92	2.81	0.11	2.88	2.86	0.02
DMAC-2Py-SO	2.90	2.87	0.03	3.06	3.02	0.05	3.10	3.07	0.03
DMAC-Ph-SO_2	2.87	2.86	0.01	3.04	3.02	0.02	3.10	3.09	0.01
DMAC-3Py-SO_2	2.34	2.33	0.01	3.32	2.93	0.39	2.59	2.58	0.01
DMAC 2Py-SO_2	2.73	2.71	0.02	3.00	2.98	0.02	2.95	2.94	0.01
DPA-Ph-SO	3.55	2.94	0.61	3.62	2.89	0.73	3.58	2.91	0.67
DPA-3Py-SO	3.66	3.04	0.62	3.74	3.00	0.74	3.71	3.04	0.67
DPA-2Py-SO	3.46	2.85	0.61	3.47	2.81	0.66	3.47	2.81	0.66
DPA-Ph-SO_2	3.32	2.79	0.53	3.55	2.80	0.75	3.44	2.82	0.62
DPA-3Py-SO_2	3.48	2.93	0.55	3.90	3.35	0.54	3.61	2.99	0.62
DPA-2Py-SO_2	3.25	2.73	0.52	3.52	2.79	0.73	3.37	2.76	0.61

Table S7. Calculated the ΔE_{ST} (in eV), oscillator strength (f), transition dipole moment (μ in debye), mean separation distance (Δr in Å), overlap extent (I in %) for vertical singlet (S_1) and triplet (T_1) energies at the M06/6-31+G* level of theory.

Molecules	**ΔE_{ST}**	**f**	**μ**	**Δr**		**I**	
				S_1	**T_1**	**S_1**	**T_1**
PXZ-Ph-SO	0.04	0.003	0.52	5.86	5.53	14.56	43.30
PXZ-3Py-SO	0.52	0.763	7.36	3.01	2.92	53.66	56.21
PXZ-2Py-SO	0.03	0.001	0.25	4.38	4.42	19.64	21.39
PXZ-Ph-SO_2	0.01	0.002	0.47	2.95	2.95	16.21	16.22
PXZ-3Py-SO_2	0.49	0.809	7.70	1.79	1.81	57.59	56.94
PXZ-2Py-SO_2	0.02	0.001	0.15	2.60	2.60	19.15	19.24
PTZ-Ph-SO	0.19	0.000	0.03	2.60	1.50	22.72	42.85
PTZ-3Py-SO	0.64	0.760	0.55	2.50	1.00	50.00	50.00
PTZ-2Py-SO	0.02	0.000	0.12	2.70	1.00	17.24	52.00

PTZ-Ph-SO_2	0.02	0.001	0.27	2.72	2.04	18.03	33.35
PTZ-3Py-SO_2	0.55	0.890	7.89	1.06	1.12	57.03	56.70
PTZ-2Py-SO_2	0.02	0.000	0.11	6.28	5.95	13.84	17.01
DMAC-Ph-SO	0.02	0.000	0.16	5.57	4.55	15.46	40.00
DMAC-3Py-SO	0.03	0.004	0.64	5.26	5.28	16.92	16.90
DMAC-2Py-SO	0.03	0.001	0.22	4.21	4.21	19.38	19.38
DMAC-Ph-SO_2	0.01	0.001	0.24	4.00	4.50	15.00	16.00
DMAC-3Py-SO_2	0.01	0.000	0.07	2.49	2.50	17.14	17.10
DMAC 2Py-SO_2	0.02	0.000	0.07	6.00	6.00	14.61	14.62
DPA-Ph-SO	0.61	0.657	6.97	1.09	1.13	52.60	53.76
DPA-3Py-SO	0.62	0.587	6.48	3.77	2.57	53.07	60.27
DPA-2Py-SO	0.61	0.382	5.40	1.95	1.28	44.30	14.62
DPA-Ph-SO_2	0.53	0.750	7.60	1.22	1.19	62.13	63.01
DPA-3Py-SO_2	0.55	0.850	7.90	1.24	1.21	62.56	61.90
DPA-2Py-SO_2	0.52	0.637	7.08	1.53	1.49	60.88	60.74

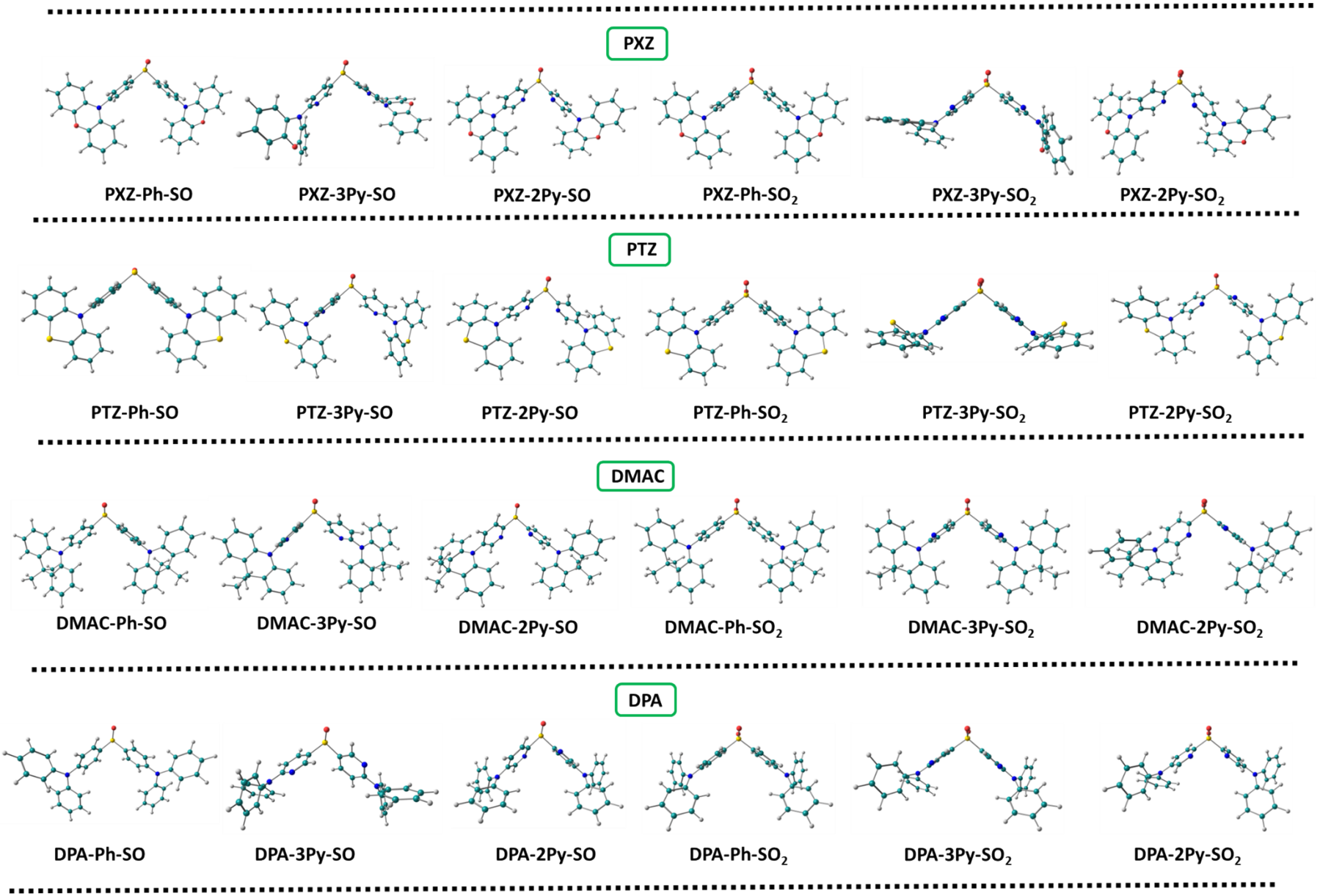

Figure S1. Optimized geometries of designed molecules using B3LYP/6-31+G* level of theory.

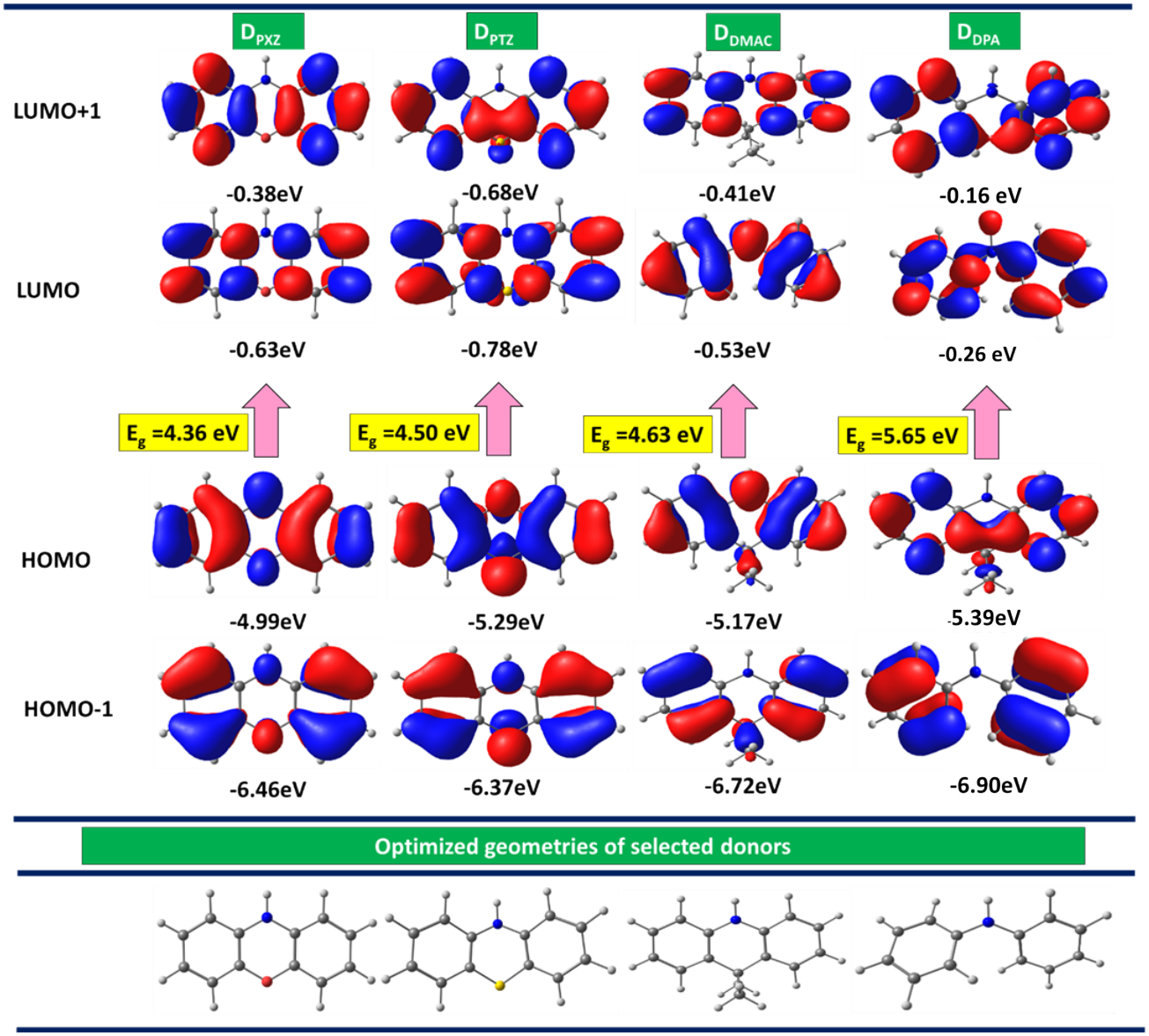

Figure S2. Frontier molecular orbital (FMOs) and optimized geometries of selected donors (iso-surface value = 0.02 au) using B3LYP/6-31+G* level of theory.

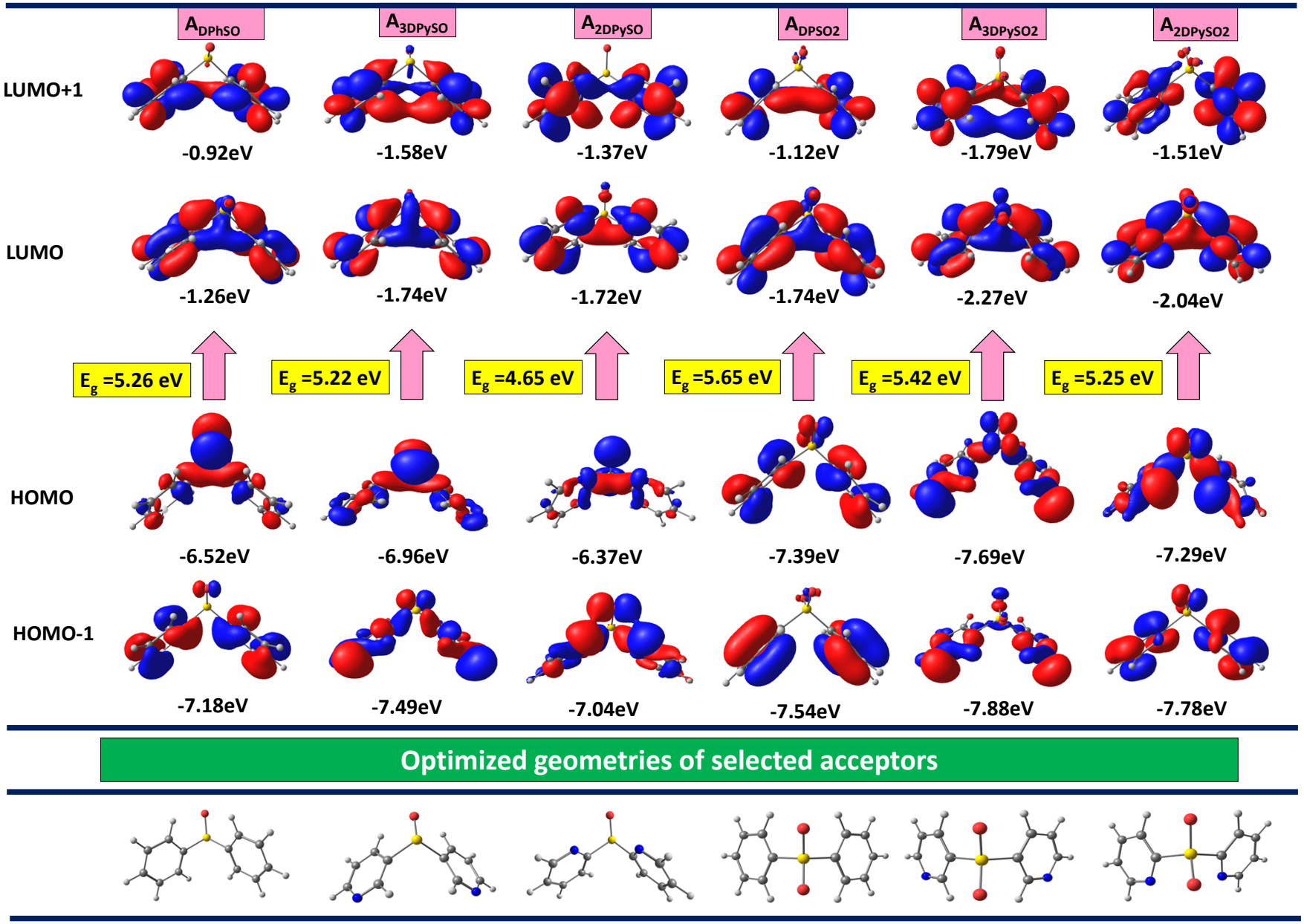

Figure S3. Frontier molecular orbital (FMOs) and optimized geometries of selected acceptors (iso-surface value = 0.02 au) using B3LYP/6-31+G* level of theory.

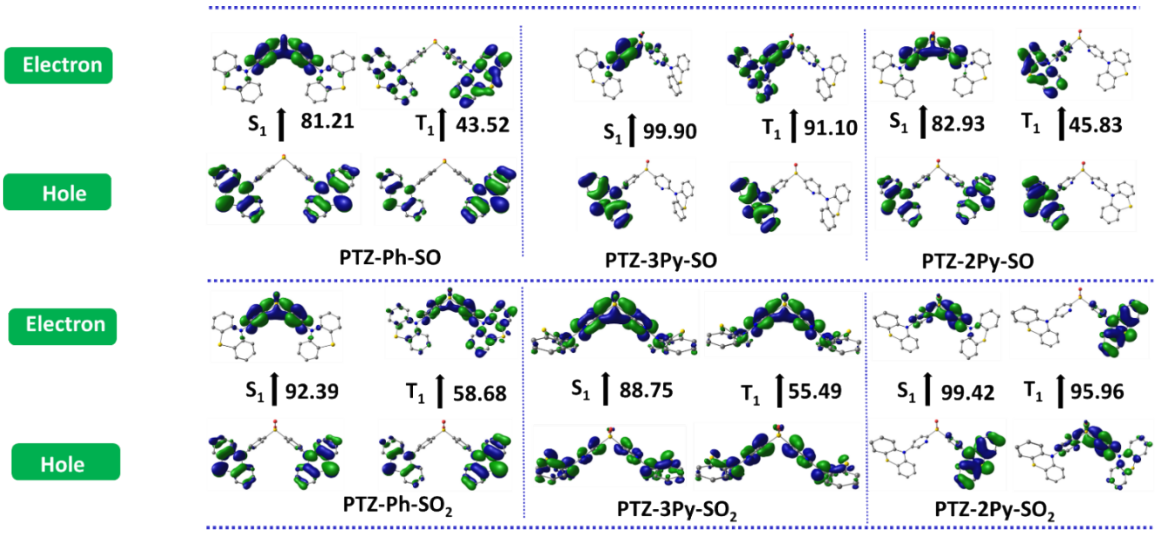

Figure S4. Natural transition orbitals (NTOs) of the S_1 and T_1 state for PTZ substituted molecules (iso-surface value = 0.02 au) at M06/6-31+G* level of theory. Hydrogen atoms are omitted for clarity.

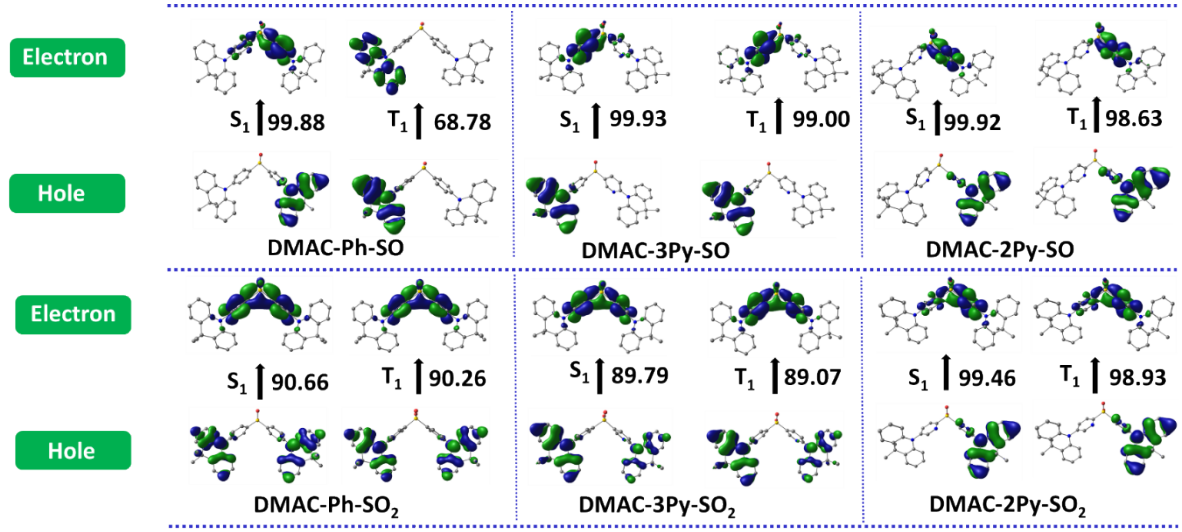

Figure S5. Natural transition orbitals (NTOs) of the S_1 and T_1 state for DMAC substituted molecules (iso-surface value = 0.02 au) at M06/6-31+G* level of theory. Hydrogen atoms are omitted for clarity.

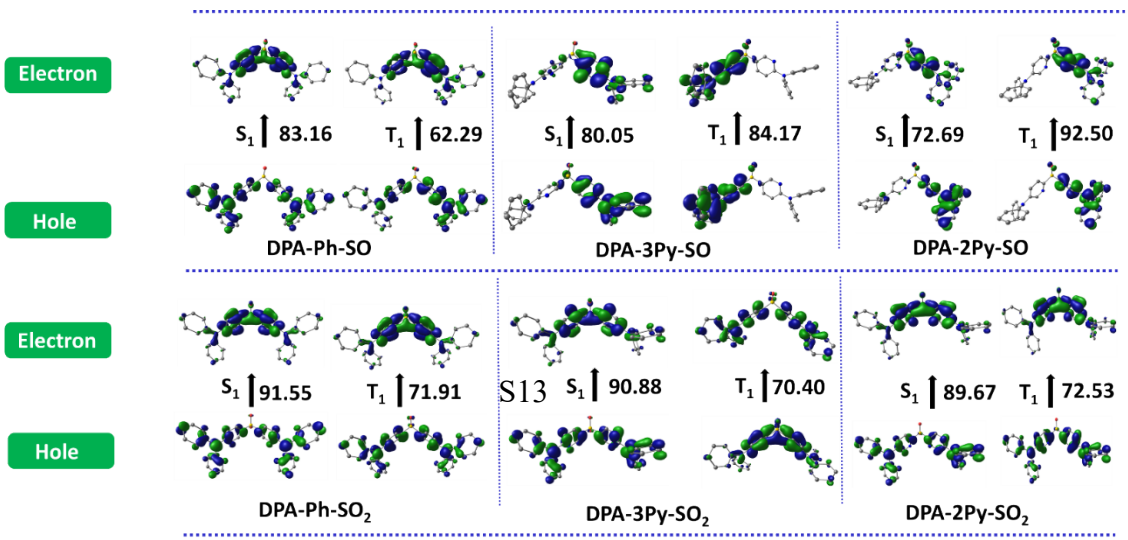

Figure S6. Natural transition orbitals (NTOs) of the S_1 and T_1 state for DPA substituted molecules (iso-surface value = 0.02 au) at M06/6-31+G* level of theory. Hydrogen atoms are omitted for clarity.

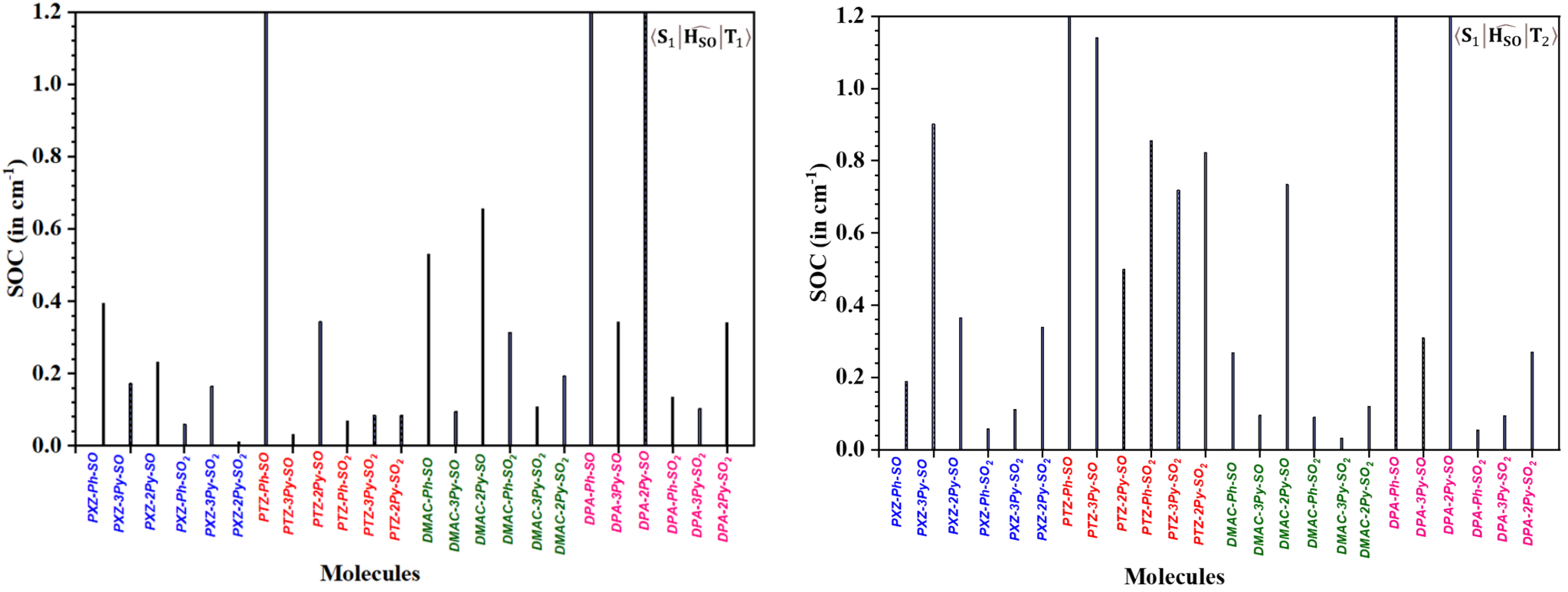

Figure S7. Spin-orbit coupling values (in cm^{-1}) between Singlet and triplet states of T_1 geometry calculated at the M06/ def2-SVP level of theory.

Spin-orbit coupling (SOC) calculations

The calculations for the spin-orbit coupling (SOC) were performed utilizing the ORCA 4.0 package. The SOC values were determined for T_1 geometries using the M06/def2-SVP level of theory. The equation is,

$$\mathbf{SOC} = \sqrt{(\langle S_n | \hat{H_{SOC}}^x | T_n \rangle^2 + \langle S_n | \hat{H_{SOC}}^y | T_n \rangle^2 + \langle S_n | \hat{H_{SOC}}^z | T_n \rangle^2)/3}$$

For instance, we provided the calculated SOC values for molecules **PXZ-Ph-SO** and **PXZ-3Py-SO**, specifically between the S_1 and T_1 states, using the optimized T_1 geometry.

Molecules	SOCx	SOCy	SOCz	x^2	y^2	z^2	$x^2 + y^2 + z^2$	$(x^2 + y^2 + z^2)/3$	SQRT $((x^2 + y^2 + z^2)/3)$
PXZ-Ph-SO	0.27	0.46	0.42	0.0729	0.2116	0.1764	0.4609	0.1536	0.39
PXZ-3Py-SO	0.23	0.11	0.15	0.0529	0.0121	0.0225	0.0875	0.0291	0.17

ISC and RISC rate calculations

The intersystem crossing (ISC) and reverse intersystem crossing rates (RISC) were calculated by using semiclassical Marcu's equation,

$$\mathbf{k} = \frac{2\pi}{\hbar} |V|^2 \frac{1}{\sqrt{4\pi k_B T \lambda}} \mathbf{exp}\left(-\frac{(\lambda + \Delta E_{ST})^2}{4\lambda k_B T}\right)$$

ħ	-	Reduced Planck's constant.
K_B	-	Boltzmann constant.
V	-	Spin-orbit coupling
T	-	Temperature.
λ	-	Reorganization energy.

The energy difference ΔE_{ST} (M06 functional) represents the variance between the relevant excited states, with opposite signs for intersystem crossing (ISC) and reverse intersystem crossing (RISC). For our rate computations, we incorporated the spin-orbit coupling (SOC) values derived from the optimized geometry of the T_1 state.

The total reorganization energy comprises both the intramolecular reorganization energy and the contribution of reorganization energy from the surrounding environment. As a result, we accounted for total reorganization energies of 0.20 eV when calculating the ISC and RISC rates. This value represents the combined effects of medium-induced relaxations, a topic that has been thoroughly discussed in prior studies.

$$\lambda\ (\text{total}) = \lambda\ (\text{surroundings}) + \lambda\ (\text{intramolecular})$$

$$\lambda\ (\text{intramolecular}) = E^{*}_{S1}\ (T_1\text{-geometry}) - E_{S1}\ (S_1\text{-geometry})$$

Where E^{*}_{S1} represents the energy of the S_1 state at the T_1-state geometry, and E_{S1} represents the energy at the S_1-state geometry. Here, we outline the calculations for the ISC and RISC rates for molecule (PXZ-Ph-SO) transition between the S_1 and T_1 states. The spin-orbit coupling (SOC) value between these states for molecule (PXZ-Ph-SO) is determined to be 0.000048354eV, while the reorganization energy (λ) is fixed at 0.20 eV.

Table S8. Calculated intramolecular reorganization energies for reference molecules at M06/6-31G* level of theory.

Molecules	E_{S1} (S_1 geometry)	E^{*}_{S1} (T_1 geometry)	λ (in Hartree)	λ (in eV)
			S_1-T_1	S_1-T_1
PXZ-Ph-SO_2	-2193.44915	-2193.44371	0.00544	0.15
PTZ-Ph-SO_2	-2839.38947	-2839.38258	0.00689	0.19
DMAC-Ph-SO_2	-2278.76428	-2278.75914	0.00514	0.14
DPA-Ph-SO_2	-2045.43937	-2045.43254	0.00683	0.19

For ISC:

$$\frac{2\pi}{\hbar}\,|H|^2\frac{1}{\sqrt{4\pi k_B T\lambda}} = 8.76\times10^{+07}\ \text{eV s}^{-1}$$

$$\exp\left(-\frac{(\lambda+\Delta E_{ST})^2}{4\lambda k_B T}\right) = 2.23766\times10^{-05} eV^{-1}$$

$$\mathbf{k\ (ISC) = 6.91\times10^{+07}\ s^{-1}}$$

For RISC:

$$\frac{2\pi}{\hbar}|V|^2\frac{1}{\sqrt{4\pi k_B T\lambda}} = 8.76*10^{+07}\ \text{eV s}^{-1}$$

$$\exp\left(-\frac{(\lambda + \Delta E_{ST})^2}{4\lambda k_B T}\right) = 2.23766*10^{-05}\text{eV}^{-1}$$

$$k\ (\text{RISC}) = 2.01 \times 10^{+03}\ \text{s}^{-1}$$

The numerical values used in ISC and RISC rate calculation:

π	-	3.141
V	-	SOC values (in eV)
ħ	-	6.5821×10^{-16} eV s
K_B	-	8.6173×10^{-5} eV K^{-1}
λ	-	0.20 eV
T	-	300 K

The optimized structure's cartesian coordinates utilizing the B3LYP/6-31+G* level of theory. (All the cartesian coordinates are in Å)

PXZ-Ph-SO

Atoms	x	y	z
C	-3.03678700	-1.06066200	1.07372400
C	-1.95467800	-1.93912200	1.14201200
C	-1.40010000	-2.42654000	-0.04159400
C	-1.93023000	-2.08402200	-1.28640000
C	-3.01338300	-1.20352000	-1.34801900
C	-3.56437400	-0.68802400	-0.16990000
H	-3.48267100	-0.66323800	1.98139400
H	-1.54684200	-2.26100500	2.09637400
H	-1.51806100	-2.50345800	-2.20130000
H	-3.44469900	-0.92124600	-2.30418600
S	-0.01200500	-3.61957600	0.05909900
C	1.36499300	-2.40502200	-0.00651200
C	2.07636900	-2.16290600	1.16745100
C	1.73653700	-1.81350100	-1.21564000
C	3.16313800	-1.28567000	1.13573600
H	1.77940900	-2.66778000	2.08264400
C	2.82047500	-0.93414300	-1.23919800
H	1.19353100	-2.02783200	-2.13304800
C	3.53361100	-0.66729200	-0.06414300
H	3.73093100	-1.07989300	2.03904300
H	3.12602300	-0.45589700	-2.16542500
O	-0.01380800	-4.16937400	1.47359400
C	5.95500600	-0.27610500	-0.28689600
C	4.48680400	1.57672900	0.28754100
C	7.03731700	0.62348500	-0.29454800
C	6.22679600	-1.63704000	-0.47496500
C	5.60622100	2.42989900	0.26673700
C	3.25532600	2.11429000	0.68267800
C	8.34010100	0.18146700	-0.47974500
C	7.53886800	-2.08461700	-0.67089900
H	5.41023500	-2.35083300	-0.47306900
C	5.50139500	3.76478500	0.63306200
C	3.14505700	3.46250100	1.04398400
H	2.37691600	1.47853800	0.70400300
C	8.59891600	-1.18067700	-0.67345800
H	9.13888000	0.91725300	-0.47656000
H	7.71934700	-3.14568400	-0.81862900
H	6.39623300	4.37930500	0.60037000
C	4.26430200	4.29170500	1.02275100
H	2.17644200	3.85252500	1.34411200
H	9.61909100	-1.52143000	-0.82357200

H	4.18614500	5.33782400	1.30368100
C	-4.45530700	1.60328900	-0.29617700
C	-5.99001900	-0.27089600	-0.04666700
C	-5.56411600	2.47035400	-0.31160100
C	-3.17502600	2.16929300	-0.34437500
C	-7.06042500	0.64284600	-0.06537900
C	-6.28332200	-1.62632300	0.14931100
C	-5.39981100	3.84754100	-0.37216800
C	-3.00689300	3.55759100	-0.41261300
H	-2.30443400	1.52256900	-0.33255600
C	-8.37066200	0.22029900	0.11344300
C	-7.60437100	-2.05579600	0.32374500
H	-5.47716000	-2.35172200	0.16200600
C	-4.11523000	4.40133000	-0.42668700
H	-6.28859900	4.47158500	-0.38080800
H	-2.00170300	3.96773100	-0.45435400
H	-9.15935800	0.96657200	0.09146800
C	-8.65149300	-1.13715600	0.30861000
H	-7.80140800	-3.11386700	0.47157300
H	-3.99258300	5.47910400	-0.47893200
H	-9.67849100	-1.46298400	0.44455300
N	4.64874100	0.23005300	-0.10546400
N	-4.67671400	0.20989000	-0.24343300
O	6.84772500	1.98597700	-0.15016600
O	-6.86133200	1.99305400	-0.28858900

PXZ-2Py-SO

Atoms	x	y	z
C	-2.67219200	-0.78696700	1.22951500
C	-1.32525700	-2.35056300	0.00608000
C	-2.11048400	-2.08067600	-1.10885900
C	-3.38012100	-0.52961100	0.02679100
H	-2.95298600	-0.30061700	2.15548700
H	-1.94198300	-2.60071400	-2.05141300
S	-0.00668600	-3.59521300	-0.08284100
C	1.42944800	-2.46829200	-0.16690600
C	1.73805200	-1.74350600	-1.31424600
C	3.41574800	-1.56874000	0.83326900
H	1.09789800	-1.78193400	-2.19512900
C	3.65073100	-0.86713000	-0.37226600
H	4.08295800	-1.46329800	1.67974900
C	5.84195900	-0.05335900	0.41211500
C	4.73120100	1.16119000	-1.32909700
C	6.25646300	1.16220300	0.97034400
C	6.52597900	-1.22427300	0.75885500

C	5.17235600	2.34805800	-0.72203800
C	4.31643800	1.20668800	-2.66515700
C	7.28774700	1.21584500	1.90518700
C	7.55304100	-1.18338600	1.70388200
H	6.23643400	-2.16451900	0.29889300
C	5.15782400	3.56310600	-1.39908400
C	4.28973400	2.42629800	-3.34801700
H	3.99087400	0.29571600	-3.14715900
C	7.92618800	0.03350300	2.28510100
H	7.57420400	2.17848800	2.31771300
H	8.06560600	-2.10084800	1.97862900
H	5.50459000	4.45431200	-0.88483800
C	4.69816400	3.60374400	-2.71728400
H	3.94839800	2.44944400	-4.37916300
H	8.72607300	0.06650400	3.01941300
H	4.67587600	4.54996400	-3.25077700
C	-4.65345000	1.30879300	1.06414600
C	-5.55195700	0.26287200	-0.89526000
C	-5.94744800	1.38473500	1.59411200
C	-3.66111100	2.15167700	1.57754600
C	-6.82462600	0.36396700	-0.31125800
C	-5.46222200	0.06387800	-2.27758600
C	-6.24409900	2.23023000	2.66068800
C	-3.94540000	2.99493400	2.65352600
H	-2.66649400	2.12889700	1.14203100
C	-7.98567900	0.21886600	-1.06349800
C	-6.62491500	-0.09074600	-3.03794800
H	-4.48720600	0.00122700	-2.73975700
C	-5.23216900	3.02541000	3.20235100
H	-7.25865300	2.25406300	3.04662300
H	-3.16368400	3.63279400	3.05595900
H	-8.94709400	0.29903000	-0.56540500
C	-7.88310900	-0.02543900	-2.43460400
H	-6.54053700	-0.26300400	-4.10725900
H	-5.45441100	3.68181700	4.03891600
H	-8.78469000	-0.14815000	-3.02831300
N	4.76641700	-0.02435700	-0.52339300
N	-4.42970000	0.40048400	-0.01257400
O	5.64406500	2.33623900	0.58272500
O	-6.95606100	0.62046100	1.04583000
C	-1.63809100	-1.70488400	1.20972600
C	2.29695400	-2.38374500	0.92484500
N	2.81901600	-0.96532900	-1.42062900
N	-3.10071300	-1.18081300	-1.11022300
H	-1.09527200	-1.95403300	2.11776600
H	2.07724300	-2.94701700	1.82803500

O	0.08205900	-4.24953700	1.28811400

PXZ-3Py-SO

Atoms	x	y	z
C	-2.42642100	-0.78573000	0.77797500
C	-1.32118500	-2.42078200	-0.35913200
C	-2.23723100	-2.41854600	-1.41107500
C	-3.30580400	-1.52319500	-1.33660500
C	-3.40703400	-0.68991000	-0.21969500
H	-2.48370000	-0.14558000	1.65595800
H	-2.11774300	-3.09023800	-2.25608500
H	-4.05248900	-1.46975900	-2.12423200
S	0.05223300	-3.66264200	-0.40826900
C	1.40623500	-2.43744700	-0.19849800
C	2.13941800	-2.44222400	0.98497100
C	2.63691500	-0.77218300	-1.13877300
C	3.18606000	-1.52524500	1.08198000
H	1.87782000	-3.13180000	1.78150900
C	3.44242400	-0.67242300	0.00241200
H	2.81999300	-0.12192300	-1.99136500
H	3.79836600	-1.46325600	1.97775700
C	4.28539100	1.54117900	0.66122700
C	5.82042900	-0.10486400	-0.26936100
C	5.35816500	2.44786800	0.74387300
C	3.04727700	1.93249200	1.18552000
C	6.85323900	0.84464200	-0.16167900
C	6.15189200	-1.39595600	-0.69826800
C	5.20150800	3.69604600	1.33125400
C	2.88451100	3.19386000	1.77085400
H	2.20338300	1.25314300	1.13355500
C	8.16745700	0.51564200	-0.46506800
C	7.47505600	-1.72805500	-1.01295900
H	5.37421800	-2.14592100	-0.79386800
C	3.95784600	4.07867800	1.84718200
H	6.06145900	4.35811400	1.37039400
H	1.91145800	3.47235700	2.16547900
H	8.92711500	1.28516100	-0.36441500
C	8.48640300	-0.77703800	-0.89696600
H	7.70220800	-2.73626800	-1.34760800
H	3.83876700	5.05808400	2.30097000
H	9.51498200	-1.02823000	-1.13831100
C	-4.40940000	1.49440600	-0.73706100
C	-5.71065200	-0.17838100	0.46741600
C	-5.51400600	2.36249100	-0.65883700
C	-3.28323700	1.92014100	-1.45225400
C	-6.78021100	0.73423400	0.51436500
C	-5.91585600	-1.46527800	0.97961200

C	-5.49644700	3.60544400	-1.27742000
C	-3.26053300	3.17588100	-2.07091200
H	-2.41553900	1.27316300	-1.52330600
C	-8.00958300	0.37383000	1.04954500
C	-7.15218100	-1.82877300	1.52665800
H	-5.10666100	-2.18731700	0.96035300
C	-4.36448800	4.02146200	-1.98775000
H	-6.37519200	4.23717500	-1.18757600
H	-2.37161300	3.48148200	-2.61540100
H	-8.80294700	1.11530000	1.06156900
C	-8.20205700	-0.91383000	1.56317400
H	-7.28102600	-2.83227000	1.92201800
H	-4.35414100	4.99654100	-2.46564900
H	-9.16379200	-1.18923400	1.98565100
N	4.49763800	0.28828800	0.04013800
N	-4.47487000	0.24515100	-0.07668800
O	6.60165700	2.15026100	0.21763400
O	-6.64862300	2.03286300	0.05836200
N	1.62996600	-1.64805100	-1.24371000
N	-1.39773000	-1.63553000	0.70990700
O	0.00333300	-4.46888500	0.87440000

PXZ-Ph-SO_2

Atoms	x	y	z
C	-3.13487100	-0.98313400	1.13420600
C	-2.02511300	-1.82795500	1.16738900
C	-1.43182500	-2.21632000	-0.03655700
C	-1.93095900	-1.78575500	-1.26768300
C	-3.03967100	-0.93781900	-1.29050800
C	-3.63962700	-0.53305800	-0.09275400
H	-3.61905100	-0.67401200	2.05614000
H	-1.63832400	-2.20281700	2.10962400
H	-1.47230300	-2.12622500	-2.19052400
H	-3.45152900	-0.59107300	-2.23373800
S	0.00002000	-3.31873100	0.00032400
C	1.43187100	-2.21633100	0.03705700
C	1.93106000	-1.78566600	1.26812700
C	2.02511800	-1.82806600	-1.16694300
C	3.03977700	-0.93773800	1.29084000
H	1.47243200	-2.12606100	2.19101000
C	3.13487000	-0.98323500	-1.13387100
H	1.63831200	-2.20300700	-2.10913900
C	3.63967600	-0.53305400	0.09303100
H	3.45168900	-0.59093500	2.23402800
H	3.61900400	-0.67418300	-2.05585300
O	-0.03419900	-4.03403800	1.28768500

O	0.03423200	-4.03421600	-1.28693300
C	6.08067600	-0.22258900	0.12682000
C	4.62472200	1.71486400	-0.10621000
C	7.18762700	0.64576000	0.10812800
C	6.32278700	-1.60158700	0.15311900
C	5.76960900	2.53354500	-0.12118800
C	3.37798500	2.32030100	-0.30758300
C	8.48660700	0.15618900	0.11406600
C	7.63184200	-2.09785400	0.16798400
H	5.48723600	-2.29298000	0.16792600
C	5.67335600	3.90137500	-0.33840900
C	3.27754900	3.70084200	-0.51814800
H	2.47958200	1.71280200	-0.29354500
C	8.71675200	-1.22416300	0.14808500
H	9.30566000	0.86913500	0.09846100
H	7.78980200	-3.17229900	0.19374200
H	6.58767100	4.48737000	-0.34153400
C	4.42151500	4.49558000	-0.53673000
H	2.29687900	4.14358700	-0.66844100
H	9.73458900	-1.60260300	0.15853400
H	4.35114700	5.56671600	-0.70116600
C	-4.62477400	1.71484100	0.10642200
C	-6.08062500	-0.22262800	-0.12719200
C	-5.76967700	2.53350500	0.12108500
C	-3.37809900	2.32028700	0.30813500
C	-7.18759900	0.64569700	-0.10877000
C	-6.32270700	-1.60163000	-0.15370200
C	-5.67349900	3.90133500	0.33833000
C	-3.27773800	3.70082800	0.51875400
H	-2.47968800	1.71279600	0.29430800
C	-8.48657000	0.15610700	-0.11518300
C	-7.63175000	-2.09791600	-0.16904100
H	-5.48714200	-2.29300900	-0.16827600
C	-4.42172000	4.49554900	0.53702900
H	-6.58781800	4.48732500	0.34121200
H	-2.29711400	4.14358300	0.66931900
H	-9.30564100	0.86903700	-0.09978500
C	-8.71668100	-1.22424500	-0.14941600
H	-7.78968700	-3.17236100	-0.19494900
H	-4.35141400	5.56668600	0.70149200
H	-9.73450700	-1.60270300	-0.16023000
N	4.77972400	0.33110600	0.13243800
N	-4.77968300	0.33109300	-0.13227200
O	7.03148200	2.02005400	0.11277400
O	-7.031484	2.019997	-0.113187

PXZ-3Py-SO_2

Atoms	x	y	z
C	-2.93817000	-0.64662500	-1.40856300
C	-1.37343200	1.12664200	-1.81987600
C	-1.96280800	1.82867200	-0.76913100
C	-3.44855600	0.11984800	-0.33064700
H	-3.37703700	-1.59983600	-1.67444000
H	-1.62048000	2.82791500	-0.51216700
S	-0.01341400	1.83561900	-2.74454900
C	1.47688200	1.29763900	-1.90770600
C	2.01644900	2.04459200	-0.86101700
C	3.29082000	-0.25061700	-1.63198700
H	1.54471700	2.97075300	-0.54230000
C	3.77002400	0.57209400	-0.58237500
H	3.80079800	-1.16535400	-1.90525300
O	-0.01337000	1.19305400	-4.07233500
O	-0.09631200	3.29836400	-2.58719800
C	5.77475800	-0.83031400	-0.26800700
C	5.12857000	0.65470500	1.49521100
C	6.08531700	-1.80253700	0.69103400
C	6.34034700	-0.93119200	-1.54392000
C	5.45512900	-0.35820100	2.40956200
C	5.04721800	1.97436800	1.95256900
C	6.88461400	-2.89919600	0.37615800
C	7.13519500	-2.03138700	-1.87230100
H	6.14185400	-0.15510800	-2.27722200
C	5.64492900	-0.08631100	3.76074300
C	5.22984800	2.25376300	3.30962800
H	4.81301000	2.76398000	1.25222400
C	7.39594300	-3.02053900	-0.91750100
H	7.09710300	-3.63433600	1.14637000
H	7.55624600	-2.10980000	-2.87049100
H	5.89142900	-0.90333800	4.43194200
C	5.51557800	1.22794900	4.21443200
H	5.14617700	3.27987100	3.65625100
H	8.01520000	-3.87601100	-1.17203100
H	5.65484100	1.44891100	5.26901500
C	-4.97500600	-1.69049100	0.35600100
C	-5.42157300	0.53377600	1.12221200
C	-6.34854600	-1.87612800	0.15555600
C	-4.15043500	-2.81366600	0.48522200
C	-6.78523900	0.29013400	0.89921200
C	-5.05517800	1.58305800	1.97178800
C	-6.89203800	-3.15084800	0.01157300
C	-4.68395800	-4.09511600	0.33388900
H	-3.09232300	-2.67627500	0.68755200
C	-7.77033400	1.09866400	1.45722500

C	-6.03906900	2.40301500	2.53073700
H	-4.00735600	1.76866900	2.16244200
C	-6.05065600	-4.26264600	0.08412500
H	-7.96085200	-3.25215500	-0.15011200
H	-4.03339900	-4.96076700	0.41933000
H	-8.81267400	0.87526300	1.25136500
C	-7.39147100	2.17177100	2.26621700
H	-5.74162300	3.22670000	3.17345100
H	-6.46655600	-5.25929900	-0.03331700
H	-8.15333800	2.81365200	2.69968000
N	4.92819200	0.24641400	0.13372500
N	-4.49900000	-0.34939300	0.46636300
O	5.60872900	-1.66827600	1.97823400
O	-7.18677200	-0.78246200	0.11572100
C	-1.89035100	-0.13280500	-2.15208200
C	2.13506900	0.12381500	-2.29557400
N	3.13237100	1.69675500	-0.21825900
N	-2.96530200	1.33795700	-0.03812200
H	1.74468900	-0.47866700	-3.11019200
H	-1.49704900	-0.67758400	-3.00508200

PXZ-2Py-SO_2

Atoms	x	y	z
C	-2.57076100	-0.47433600	0.87110300
C	-1.42547000	-2.18093000	-0.09846400
C	-2.33109900	-2.32169700	-1.14731500
C	-3.43296400	-1.46526800	-1.14739100
C	-3.55891200	-0.52347800	-0.12149200
H	-2.64408000	0.25465400	1.67490200
H	-2.16710400	-3.06227900	-1.92240700
H	-4.18352700	-1.51715600	-1.93127600
S	-0.00009200	-3.31809600	0.00038800
C	1.42532200	-2.18096500	0.09904100
C	2.33097900	-2.32157300	1.14786900
C	2.57057200	-0.47451800	-0.87082900
C	3.43289100	-1.46516900	1.14775900
H	2.16700500	-3.06201100	1.92310400
C	3.55879900	-0.52355000	0.12171200
H	2.64387300	0.25437300	-1.67472100
H	4.18349400	-1.51698500	1.93161000
O	-0.05285500	-4.04777100	1.27750800
O	0.05266300	-4.04792700	-1.27663800
C	4.63004800	1.56656100	0.84441500
C	5.88926600	-0.03914600	-0.48905400
C	5.76320200	2.40036400	0.85020900

C	3.51534700	1.95951600	1.59518300
C	6.98841700	0.83771300	-0.44709300
C	6.06033500	-1.28644000	-1.10165700
C	5.78366800	3.57999200	1.58226100
C	3.53080900	3.15239800	2.32790100
H	2.62699700	1.33717700	1.60570300
C	8.21446300	0.47983000	-0.99153600
C	7.29327300	-1.64651700	-1.65854900
H	5.22774000	-1.97974700	-1.15337600
C	4.66214200	3.96526700	2.32562600
H	6.68326700	4.18763900	1.55395900
H	2.65021600	3.43464200	2.89788600
H	9.03175300	1.19245800	-0.93227600
C	8.37319800	-0.76809200	-1.60498600
H	7.39594400	-2.61861100	-2.13222400
H	4.68124500	4.89134700	2.89243200
H	9.33251000	-1.04139500	-2.03425400
C	-4.62966000	1.56693200	-0.84405800
C	-5.88961800	-0.03904900	0.48838000
C	-5.76273600	2.40084100	-0.85011900
C	-3.51459700	1.95999000	-1.59423900
C	-6.98868500	0.83790400	0.44614200
C	-6.06104900	-1.28646100	1.10064200
C	-5.78275100	3.58069600	-1.58181600
C	-3.52960800	3.15310300	-2.32659200
H	-2.62632300	1.33754100	-1.60459400
C	-8.21500600	0.47997500	0.98993200
C	-7.29427100	-1.64658900	1.65687300
H	-5.22852000	-1.97982900	1.15260700
C	-4.66085300	3.96609300	-2.32455600
H	-6.68230600	4.18841800	-1.55374200
H	-2.64874200	3.43541600	-2.89612100
H	-9.03221300	1.19268300	0.93048300
C	-8.37411700	-0.76808500	1.60300400
H	-7.39721700	-2.61878000	2.13029200
H	-4.67961400	4.89235200	-2.89108100
H	-9.33364800	-1.04142400	2.03175700
N	4.65852500	0.38332300	0.06840500
N	-4.65860000	0.38344700	-0.06844500
O	6.88897200	2.10085800	0.10622300
O	-6.88889000	2.10119400	-0.10677600
N	1.51598700	-1.29587500	-0.88591900
N	-1.51617600	-1.29570400	0.88634900

PTZ-Ph-SO

Atoms	x	y	z
C	3.12110400	-1.28135200	-1.13819400
C	2.02906900	-2.15131300	-1.15755300
C	1.38550600	-2.46090200	0.03979300
C	1.83350900	-1.94473400	1.25671700
C	2.92306200	-1.07135900	1.26792600
C	3.56853100	-0.73576400	0.07263400
H	3.63496700	-1.02818300	-2.06162200
H	1.68050200	-2.60366700	-2.08203200
H	1.35001600	-2.21872600	2.19142700
H	3.28954900	-0.65316300	2.20086100
S	-0.00001600	-3.66345800	-0.00393800
C	-1.38553700	-2.46091000	0.03981700
C	-2.02897600	-2.15112300	-1.15754500
C	-1.83366400	-1.94493600	1.25677900
C	-3.12100200	-1.28115300	-1.13815800
H	-1.68032700	-2.60333800	-2.08206200
C	-2.92320900	-1.07155000	1.26801600
H	-1.35027700	-2.21909600	2.19149400
C	-3.56854600	-0.73575200	0.07271200
H	-3.63476800	-1.02783100	-2.06159800
H	-3.28979200	-0.65350600	2.20098200
C	-6.00131800	-0.41155500	0.13699400
C	-4.49269400	1.52477700	-0.19347600
C	-7.10697900	0.36970300	0.52892200
C	-6.23099300	-1.75045000	-0.22130800
C	-5.45923500	2.48532000	0.16758200
C	-3.33444200	1.96827900	-0.85348700
C	-8.39791800	-0.16385500	0.51310100
C	-7.51973400	-2.28918100	-0.19424700
H	-5.40096300	-2.38305500	-0.51256100
C	-5.28751100	3.83030900	-0.16851300
C	-3.15033500	3.32137900	-1.14846200
H	-2.56401400	1.25829200	-1.12955100
C	-8.61179200	-1.49884400	0.16301000
H	-9.23306000	0.47030300	0.79887600
H	-7.66156600	-3.33169300	-0.46627000
H	-6.06131200	4.54348700	0.10329100
C	-4.12798000	4.25930700	-0.81805200
H	-2.23793900	3.63292700	-1.65000000
C	4.49274700	1.52469200	-0.19392100
C	6.00129900	-0.41157900	0.13721600
C	5.45924400	2.48530500	0.16706700
C	3.33460000	1.96805800	-0.85420800
C	7.10690800	0.36975300	0.52914600
C	6.23101800	-1.75055400	-0.22076100

C	5.28759100	3.83021900	-0.16936500
C	3.15055700	3.32109200	-1.14952300
H	2.56420400	1.25801700	-1.13022400
C	8.39784400	-0.16382100	0.51364400
C	7.51974900	-2.28929200	-0.19338000
H	5.40102800	-2.38321300	-0.51201000
C	4.12816500	4.25908300	-0.81918100
H	6.06136100	4.54344800	0.10239400
H	2.23824300	3.63253700	-1.65127400
H	9.23294700	0.47039000	0.79941000
C	8.61175900	-1.49888800	0.16387800
H	7.66161500	-3.33186400	-0.46515700
N	-4.69593800	0.15429700	0.12731000
N	4.69592500	0.15428500	0.12720800
S	-6.85169200	2.01083600	1.17022700
S	6.85153600	2.01103300	1.17004000
H	-3.99439200	5.31028700	-1.05772500
H	-9.61690300	-1.91057700	0.17248800
H	3.99462800	5.31000900	-1.05911900
H	9.61686400	-1.91063000	0.17360500
O	-0.00001700	-4.25703300	-1.40127900

PTZ-3Py-SO

Atoms	x	y	z
C	-3.17451900	-1.50914700	1.26059300
C	-1.34809100	-2.49245400	0.07984900
C	-1.73960600	-1.76708000	-1.04766800
C	-3.47318400	-0.79177900	0.09426600
H	-3.79364500	-1.38904800	2.14447900
H	-1.20584800	-1.85519700	-1.99273800
S	0.03835200	-3.69385500	0.02971600
C	1.41207600	-2.48351100	0.02604100
C	1.93768800	-2.00072700	-1.17303600
C	3.06784600	-1.21580200	1.18480200
H	1.52920200	-2.30916300	-2.13437400
C	3.51490300	-0.76057700	-0.06504000
H	3.55805600	-0.87444000	2.09155000
C	5.93253400	-0.33000600	-0.04124900
C	4.30572200	1.54963700	-0.10628200
C	7.02037200	0.45309000	-0.47753700
C	6.20627800	-1.59842400	0.49739200
C	5.24279700	2.50094000	-0.55443700
C	3.07681200	2.01386400	0.39165500
C	8.33171200	-0.00367700	-0.32347600
C	7.51805800	-2.06607200	0.60745800
H	5.39490000	-2.23928600	0.82194300

C	4.96613100	3.86738700	-0.46349700
C	2.78950500	3.37995000	0.43791400
H	2.32856800	1.30822100	0.73439600
C	8.58983000	-1.26833000	0.20944400
H	9.15076300	0.63263300	-0.64842900
H	7.69221100	-3.05762900	1.01652800
H	5.71690300	4.57890900	-0.79726100
C	3.73498100	4.31562200	0.01975400
H	1.82237400	3.70474000	0.81204400
H	9.61246100	-1.62145400	0.30561300
H	3.52173400	5.37970200	0.06448600
C	-4.45907800	1.39572500	0.64423600
C	-5.83385900	-0.39654500	-0.38888900
C	-5.33923400	2.43251300	0.27225600
C	-3.46996800	1.68131500	1.60024500
C	-6.83357100	0.47479900	-0.86154900
C	-6.11350400	-1.77252700	-0.35456300
C	-5.25760300	3.68729000	0.88148100
C	-3.36685400	2.95168700	2.17227500
H	-2.76210200	0.91597400	1.89561700
C	-8.08059900	-0.02048400	-1.25122200
C	-7.34685300	-2.26518800	-0.78648100
H	-5.36246000	-2.46932400	0.00081800
C	-4.26605100	3.95941600	1.82625900
H	-5.96492400	4.45939400	0.59022900
H	-2.58270800	3.14085000	2.90060900
H	-8.84092900	0.67730800	-1.59219300
C	-8.34027600	-1.39244600	-1.23009100
H	-7.52719600	-3.33648900	-0.76163700
H	-4.19942700	4.94446500	2.27900300
H	-9.30570100	-1.76907500	-1.55556500
N	4.60527600	0.16193300	-0.16132600
N	-4.58137800	0.11242700	0.04821100
C	-2.08692500	-2.38144800	1.25471300
C	1.99791500	-2.10567700	1.23280400
N	2.96697200	-1.14696300	-1.22001200
N	-2.77608300	-0.92334400	-1.03951000
H	-1.81420900	-2.97525300	2.12327300
H	1.62550000	-2.51138300	2.16988500
O	0.05326900	-4.34917900	1.39861200
S	-6.47996200	2.20561600	-1.07561000
S	6.74064100	1.97465000	-1.35780900
C	-3.17451900	-1.50914700	1.26059300

PTZ-2Py-SO

Atoms	x	y	z
C	-2.71839100	-1.12570000	0.95987000

C	-1.38445700	-2.44623200	-0.32394300
C	-2.08116500	-2.16556600	-1.49798400
C	-3.16194700	-1.28928700	-1.39787600
C	-3.49184600	-0.75400900	-0.14876800
H	-2.95362800	-0.73700900	1.94855400
H	-1.78201800	-2.62856100	-2.43325400
H	-3.75404400	-1.01997000	-2.26823100
S	-0.00007700	-3.67062500	-0.39985300
C	1.38437300	-2.44628600	-0.32406600
C	2.08156100	-2.16641600	-1.49801300
C	2.71798200	-1.12514100	0.95945100
C	3.16245400	-1.29026000	-1.39801400
H	1.78269800	-2.62992700	-2.43311700
C	3.49193300	-0.75425400	-0.14911000
H	2.95282400	-0.73579800	1.94797200
H	3.75494100	-1.02158100	-2.26830000
C	5.86483300	-0.40476400	0.37150700
C	4.36684100	1.53638200	0.01458900
C	7.04932500	0.31702200	0.12607700
C	5.96690200	-1.65524600	1.00193500
C	5.41405000	2.43768800	-0.26224400
C	3.09985200	2.06275100	0.31383800
C	8.28613700	-0.18430200	0.53928500
C	7.21127600	-2.16941300	1.37464100
H	5.07556000	-2.24044700	1.19588900
C	5.20208400	3.81692000	-0.19465100
C	2.88537800	3.44302600	0.33808200
H	2.27006300	1.39670600	0.51940500
C	8.37627400	-1.43504700	1.15397500
H	9.18116400	0.40443200	0.35633300
H	7.25864700	-3.14550000	1.84972300
H	6.03415500	4.48789700	-0.39108400
C	3.93493100	4.32823600	0.09361400
H	1.89104300	3.81951100	0.56259900
H	9.34428400	-1.82601700	1.45375400
H	3.77491700	5.40210100	0.12475900
C	-4.36665800	1.53657600	0.01647900
C	-5.86502600	-0.40478200	0.37066600
C	-5.41363500	2.43819700	-0.26020100
C	-3.09983000	2.06259900	0.31701600
C	-7.04931100	0.31729600	0.12511900
C	-5.96757200	-1.65582600	0.99990700
C	-5.20163200	3.81735600	-0.19122800
C	-2.88529500	3.44283900	0.34266200
H	-2.27021200	1.39632400	0.52252400
C	-8.28642300	-0.18434300	0.53705200

C	-7.21221600	-2.17026900	1.37132000
H	-5.07637800	-2.24122500	1.19394500
C	-3.93463400	4.32833500	0.09831500
H	-6.03353700	4.48855800	-0.38759000
H	-1.89108800	3.81906000	0.56818900
H	-9.18130300	0.40459500	0.35403900
C	-8.37703100	-1.43564500	1.15053500
H	-7.25995700	-3.14677100	1.84551200
H	-3.77457300	5.40216100	0.13054200
H	-9.34526100	-1.82683700	1.44931100
N	4.60898300	0.13455800	-0.02924200
N	-4.60887100	0.13481100	-0.02876800
N	1.68031200	-1.96673700	0.87741900
N	-1.68078800	-1.96736900	0.87772100
O	-0.00010500	-4.19299600	-1.82800800
S	-6.98828400	1.82465800	-0.82097600
S	6.98901100	1.82351800	-0.82144200

PTZ-Ph-SO_2

Atoms	x	y	z
C	3.10041300	-1.05053400	-1.15111700
C	1.98659600	-1.89051800	-1.15029800
C	1.43353100	-2.28421900	0.07081400
C	1.97788100	-1.86211500	1.28523100
C	3.09128200	-1.02011700	1.27364100
C	3.65282200	-0.60962500	0.05976500
H	3.55095400	-0.74111800	-2.08993800
H	1.56623500	-2.25787000	-2.08110600
H	1.55106700	-2.20593100	2.22197300
H	3.53914500	-0.68152800	2.20314600
S	-0.00001200	-3.38440300	0.07724300
C	-1.43357300	-2.28424100	0.07091600
C	-1.98627600	-1.88993000	-1.15016800
C	-1.97828900	-1.86275400	1.28537800
C	-3.10008400	-1.04994500	-1.15090200
H	-1.56564100	-2.25680200	-2.08104300
C	-3.09170700	-1.02076900	1.27387500
H	-1.55173900	-2.20704200	2.22206600
C	-3.65287700	-0.60966300	0.06004100
H	-3.55033100	-0.74003500	-2.08970000
H	-3.53985900	-0.68266200	2.20341600
O	-0.00004000	-4.10679500	-1.20715300
O	0.00002400	-4.09348300	1.36833200
C	-6.09005100	-0.34639000	-0.03713300
C	-4.61443300	1.64307300	-0.12607900

C	-7.24288500	0.38158400	0.31880400
C	-6.25372900	-1.66325100	-0.49770700
C	-5.63269000	2.55418000	0.22063500
C	-3.42244400	2.15663800	-0.66368800
C	-8.51330200	-0.17998500	0.17041800
C	-7.52513100	-2.23280300	-0.60337600
H	-5.38728300	-2.25684500	-0.76409900
C	-5.47388500	3.92224000	-0.01318600
C	-3.25484300	3.53044700	-0.85501700
H	-2.61259600	1.48574800	-0.92426600
C	-8.66240400	-1.49352400	-0.28003200
H	-9.38516700	0.41392300	0.43187600
H	-7.61651600	-3.25836300	-0.95073400
H	-6.28599000	4.59739700	0.24346400
C	-4.28114300	4.42082600	-0.54154400
H	-2.31599400	3.89620700	-1.26226200
C	4.61448300	1.64298300	-0.12738700
C	6.09003100	-0.34644800	-0.03656300
C	5.63265100	2.55428800	0.21927700
C	3.42281100	2.15626100	-0.66585700
C	7.24271300	0.38168900	0.31952000
C	6.25388300	-1.66355800	-0.49636400
C	5.47401700	3.92216700	-0.01547500
C	3.25535700	3.52999800	-0.85813000
H	2.61302200	1.48529700	-0.92642500
C	8.51318800	-0.17999100	0.17204100
C	7.52531800	-2.23319900	-0.60112100
H	5.38754100	-2.25725900	-0.76285800
C	4.28151900	4.42049800	-0.54473900
H	6.28598800	4.59750100	0.24113600
H	2.31669900	3.89548000	-1.26606400
H	9.38494500	0.41403700	0.43358500
C	8.66246000	-1.49377700	-0.27762800
H	7.61684800	-3.25894500	-0.94789200
N	-4.80351000	0.24985000	0.09049400
N	4.80345600	0.24989800	0.09014100
S	-7.08290200	1.98278000	1.08025600
S	7.08236700	1.98330700	1.07999700
H	9.65338700	-1.92888400	-0.36980400
H	4.16033400	5.48788700	-0.70517900
H	-4.15975000	5.48829700	-0.70128300
H	-9.653302	-1.928547	-0.372913

PTZ-3Py-SO_2

Atoms	x	y	z

C	-3.12503800	1.01536300	1.09711100
C	-1.42866600	-0.47168300	1.91913700
C	-1.99509400	-1.47711200	1.13583000
C	-3.61028200	-0.05630800	0.30610600
H	-3.62028300	1.97813700	1.09949700
H	-1.59082500	-2.48609800	1.15544500
S	-0.00005100	-0.80683400	2.94612800
C	1.42860900	-0.47171000	1.91918900
C	1.99513100	-1.47718400	1.13601200
C	3.12496300	1.01533800	1.09713300
H	1.59090500	-2.48618600	1.15569500
C	3.61030200	-0.05638300	0.30624500
H	3.62017500	1.97812900	1.09947100
O	-0.00006400	0.20097700	4.02360000
O	-0.00006400	-2.25230400	3.23226500
C	-2.02261200	0.79718700	1.90477400
C	2.02250200	0.79718700	1.90474900
N	3.05080300	-1.27683500	0.34557300
N	-3.05072900	-1.27674100	0.34535100
N	4.71304000	0.10046000	-0.53678900
C	5.33581700	1.37512800	-0.71874400
C	5.45085900	-1.02830800	-1.03116200
C	6.67980800	1.53642800	-0.34672200
C	4.64490000	2.44547900	-1.29950600
C	6.81064100	-1.12823900	-0.69786800
C	4.86986800	-1.99365100	-1.85977500
C	7.30850400	2.77669400	-0.51181100
S	7.56147300	0.13674200	0.31843000
C	5.26632400	3.68653100	-1.44189600
H	3.61752100	2.29983100	-1.62134700
C	7.57321300	-2.20622200	-1.16171800
C	5.62692500	-3.07784200	-2.30422100
H	3.82363900	-1.90315800	-2.12553400
C	6.59584000	3.85443700	-1.03870000
H	8.35286000	2.88938300	-0.23410800
H	4.71843600	4.51644000	-1.87949300
H	8.62845700	-2.26555300	-0.90994500
C	6.97491000	-3.19018000	-1.94911400
H	5.16283800	-3.83368400	-2.93171800
N	-4.71294600	0.10055600	-0.53702800
C	-5.45060900	-1.02824200	-1.03156500
C	-5.33599100	1.37514700	-0.71863800
C	-6.81035900	-1.12851100	-0.69812800
C	-4.86952700	-1.99328100	-1.86041400
C	-6.67996500	1.53611500	-0.34640800
C	-4.64533900	2.44574000	-1.29925900
C	-7.57274600	-2.20653300	-1.16211200
S	-7.56128600	0.13611500	0.31854000

C	-5.62642300	-3.07755500	-2.30501600
H	-3.82334200	-1.90256000	-2.12627700
C	-7.30890700	2.77630300	-0.51114600
C	-5.26700800	3.68671100	-1.44130300
H	-3.61797500	2.30033700	-1.62125800
C	-6.97432300	-3.19022800	-1.94979400
H	-8.62795600	-2.26616400	-0.91026300
H	-5.16221700	-3.83315800	-2.93270900
H	-8.35324800	2.88874800	-0.23328700
C	-6.59650100	3.85428600	-1.03789600
H	-4.71933200	4.51681800	-1.87879200
H	-1.64125400	1.58558300	2.54669900
H	1.64108200	1.58562200	2.54658800
H	-7.08648800	4.81683400	-1.15625000
H	-7.56511500	-4.03182800	-2.30116300
H	7.08563800	4.81704800	-1.15732100
H	7.56578900	-4.03175600	-2.30039400

PTZ-2Py-SO_2

Atoms	x	y	z
C	-2.94232200	-1.18053900	0.91317500
C	-1.48421800	-2.18680400	-0.50914300
C	-2.07142100	-1.63204500	-1.64667700
C	-3.16673800	-0.79006300	-1.44888200
C	-3.61406300	-0.55239900	-0.14708900
H	-3.27073200	-1.02556200	1.93878200
H	-1.69513600	-1.86527900	-2.63663700
H	-3.67845200	-0.32321800	-2.28559900
S	-0.05731400	-3.31342900	-0.72541800
C	1.40639000	-2.22073100	-0.60589900
C	2.42469700	-2.37309400	-1.54606400
C	2.51775200	-0.61205700	0.55567000
C	3.56169000	-1.58055900	-1.38179700
H	2.32118800	-3.07660900	-2.36501700
C	3.61710600	-0.68218000	-0.31319300
H	2.52421800	0.08229800	1.39318200
H	4.39981700	-1.64703500	-2.06963900
O	-0.02216400	-4.26664000	0.38742600
O	-0.09868600	-3.77672500	-2.12764000
C	5.76427900	-0.28575600	0.80536000
C	4.74373500	1.47880900	-0.60736200
C	7.06234900	0.25755200	0.74589500
C	5.48967200	-1.24839900	1.78970500
C	5.94897500	2.18405700	-0.79493400
C	3.53826400	2.12900000	-0.91685600
C	8.03518900	-0.12375400	1.67320600
C	6.47986100	-1.65574300	2.68729500

H	4.50490500	-1.69617100	1.85570500
C	5.93516300	3.50995100	-1.23494900
C	3.53486300	3.44120900	-1.39678000
H	2.59394600	1.61101400	-0.79628100
C	7.75404700	-1.09084300	2.64069500
H	9.02200300	0.32816800	1.61771000
H	6.24020200	-2.41183000	3.42985300
H	6.87889800	4.03663700	-1.34929800
C	4.73053400	4.14231200	-1.55023400
H	2.58630300	3.91275300	-1.63903800
C	-4.49873700	1.65542800	0.46665300
C	-6.02474300	-0.28263800	0.22178400
C	-5.51407100	2.61895000	0.30605900
C	-3.26859000	2.06818300	1.00312900
C	-7.17927600	0.50252400	0.03762100
C	-6.18552200	-1.64073700	0.53884600
C	-5.31070900	3.93996200	0.71279100
C	-3.05854400	3.40025500	1.36872300
H	-2.46298300	1.35451500	1.13091100
C	-8.45007300	-0.05227600	0.20798300
C	-7.46005100	-2.19855800	0.66632400
H	-5.31723700	-2.27439400	0.67820800
C	-4.07897600	4.34141900	1.23440000
H	-6.11941600	4.65689600	0.59825800
H	-2.09250900	3.69107000	1.77251100
H	-9.32354300	0.58190700	0.08160500
C	-8.59824000	-1.40768700	0.51018100
H	-7.55288300	-3.25546400	0.90056000
N	4.77638000	0.13706000	-0.13114600
N	-4.73668000	0.30791300	0.07214000
N	1.42800200	-1.37324100	0.41602400
N	-1.89021500	-1.98447300	0.73691500
S	7.50773800	1.34882700	-0.58893900
S	-7.02563900	2.18394900	-0.52884800
H	-3.92384200	5.37481900	1.53067700
H	-9.59048100	-1.83531100	0.62119800
H	4.73131100	5.16681900	-1.91090700
H	8.52262500	-1.39595800	3.34488900

DMAC-Ph-SO

Atoms	x	y	z
C	3.02053000	-1.33401600	-1.08996300
C	1.94007200	-2.21606600	-1.10512900
C	1.39899500	-2.64910000	0.10603500
C	1.94249900	-2.24679000	1.32628300
C	3.02345400	-1.36073300	1.33352300
C	3.56202700	-0.90027200	0.12861200

H	3.45439000	-0.98038600	-2.02121800
H	1.52322800	-2.58302500	-2.03912300
H	1.54126900	-2.62238400	2.26481200
H	3.46287100	-1.03163500	2.27070000
S	0.01203400	-3.84602100	0.07909800
C	-1.36652900	-2.63235800	0.08163300
C	-2.08565500	-2.45896200	-1.10001000
C	-1.73314500	-1.97214000	1.25565600
C	-3.17321600	-1.58286900	-1.11267700
H	-1.79312200	-3.01501300	-1.98652100
C	-2.81933800	-1.09502000	1.23381600
H	-1.18457600	-2.13113400	2.18100600
C	-3.54024900	-0.89585400	0.05114700
H	-3.74515200	-1.43149100	-2.02402600
H	-3.12018500	-0.56556900	2.13321600
C	-5.96484500	-0.52294300	0.19309500
C	-4.49062900	1.31381800	-0.45447900
C	-7.05443900	0.36800600	0.32643000
C	-6.19026200	-1.91096600	0.19130800
C	-5.55331900	2.23875600	-0.33396000
C	-3.29202200	1.70165800	-1.07943600
C	-8.34466800	-0.17239900	0.38125200
C	-7.48574200	-2.41842800	0.27770700
H	-5.35588800	-2.59778500	0.11173700
C	-5.39657700	3.50244900	-0.91549400
C	-3.15676300	2.97833600	-1.62265200
H	-2.46622300	1.00390800	-1.15235100
C	-8.57383900	-1.55020600	0.35468500
H	-9.19813600	0.49150400	0.46513600
H	-7.63668200	-3.49490300	0.27120700
H	-6.20499800	4.22263000	-0.85234800
C	-4.21685900	3.88161700	-1.56053200
H	-2.22288800	3.25464700	-2.10568900
C	4.43317500	1.39162800	0.00543800
C	5.98008700	-0.49893800	-0.05729500
C	5.50928700	2.29729200	0.14885100
C	3.14581100	1.87404300	-0.29089300
C	7.08490800	0.37192600	0.08387000
C	6.18856700	-1.84378900	-0.41154600
C	5.26263000	3.65557200	-0.08364900
C	2.92717800	3.23677200	-0.48676400
H	2.31356900	1.18557400	-0.37830100
C	8.35911600	-0.12717600	-0.21139300
C	7.47382500	-2.31751900	-0.67021400
H	5.34760100	-2.52190600	-0.49551500
C	3.98991000	4.13515000	-0.40262400

H	6.07605400	4.36772700	0.00230400
H	1.92396200	3.58703800	-0.71601500
H	9.22046500	0.52655400	-0.12851100
C	8.56665600	-1.45565100	-0.59017500
H	7.61059900	-3.36009000	-0.94573600
N	-4.65824000	0.00510000	0.05763200
N	4.67528900	0.00571300	0.16107500
H	9.57107700	-1.81036700	-0.80415900
H	3.83391100	5.19766400	-0.56757000
H	-4.12774300	4.87395600	-1.99389200
H	-9.58874200	-1.93450000	0.40747300
C	-6.76531300	1.86004600	0.52441000
C	6.85213000	1.77035100	0.66649500
C	6.74776200	1.63269600	2.21655300
H	7.683093	1.231925	2.625552
H	6.55476	2.611488	2.67209
H	5.93457	0.957806	2.502214
C	8.014049	2.731968	0.356282
H	7.845069	3.708678	0.819356
H	8.95275	2.355595	0.773509
H	8.147364	2.8776	-0.721683
C	-6.381673	2.080478	2.019921
H	-6.141302	3.135555	2.198294
H	-7.216054	1.794142	2.671518
H	-5.509783	1.480583	2.299581
C	-7.993187	2.737442	0.219114
H	-8.829931	2.476862	0.87404
H	-7.774551	3.792463	0.409234
H	-8.32169	2.633342	-0.821206
O	0.007846	-4.476659	-1.301877

DMAC-3Py-SO

Atoms	x	y	z
C	3.20576200	-1.64454500	-1.26964100
C	1.36549500	-2.64657400	-0.12657400
C	1.73685300	-1.93382600	1.01563200
C	3.49009900	-0.95106500	-0.08751300
H	3.83150800	-1.49733500	-2.14439100
H	1.18571700	-2.03178200	1.94981300
S	-0.02074400	-3.84956100	-0.11139000
C	-1.39549100	-2.64154900	-0.08520900
C	-1.94659400	-2.21812400	1.12474700
C	-3.02897700	-1.32140300	-1.21747800
H	-1.55787800	-2.57425900	2.07786900
C	-3.49898400	-0.92517800	0.04268500

H	-3.50791700	-0.94052700	-2.11409200
O	-0.02699300	-4.47525400	-1.49392200
C	2.11960300	-2.51840800	-1.29050100
C	-1.95719400	-2.20743800	-1.28526500
N	-2.97808000	-1.36743600	1.19112600
N	2.77565800	-1.09205400	1.03487800
H	1.85532400	-3.09626800	-2.17222900
H	-1.56656700	-2.56971800	-2.23261500
C	-5.90985200	-0.52308800	0.09187300
C	-4.33402200	1.36164600	0.27156000
C	-7.01516100	0.35270200	0.09069500
C	-6.12228100	-1.91637400	0.05277100
C	-5.39264500	2.29316300	0.28057600
C	-3.00422900	1.81414500	0.39148400
C	-8.29684100	-0.21316500	0.02611700
C	-6.86460900	1.87872800	0.15066000
C	-7.40818700	-2.44334500	-0.01006700
H	-5.27763600	-2.59490400	0.08285100
C	-5.06629300	3.65197400	0.40073300
C	-2.71689700	3.16997000	0.51087600
H	-2.18833100	1.10119100	0.40608300
C	-8.51153300	-1.58938100	-0.02869800
H	-9.16051400	0.44563200	0.01620100
H	-7.54117700	-3.52173700	-0.03889400
H	-5.86804200	4.38493200	0.40347900
C	-3.75289400	4.10473900	0.51383700
H	-1.68227900	3.48882000	0.60786900
H	-9.52215800	-1.98462200	-0.07924300
H	-3.54551100	5.16712800	0.60587000
C	4.39089900	1.29980100	-0.39669400
C	5.85049700	-0.52215700	0.38763900
C	5.46822100	2.20994700	-0.40364700
C	3.10022600	1.74362300	-0.75083700
C	6.97088900	0.33393600	0.40655200
C	5.99053200	-1.86481400	0.79417500
C	5.20348400	3.53348400	-0.78467300
C	6.89814200	1.80632900	-0.01980000
C	2.87370800	3.06437600	-1.12431200
H	2.26453200	1.05395000	-0.72609300
C	8.19647300	-0.20269700	0.82752000
C	7.22188800	-2.36385500	1.20607800
H	5.12922500	-2.52247700	0.79848800
C	3.93157900	3.97398600	-1.14698500
H	6.02204300	4.24749600	-0.80081300
H	1.86808800	3.37718600	-1.39361700
H	9.07173600	0.44051400	0.84464400

C	8.34139400	-1.53109800	1.22393600
H	7.29907400	-3.40302500	1.51537200
H	3.77183600	5.00865000	-1.43696600
H	9.31021700	-1.90530000	1.54254200
N	-4.59659000	-0.01501000	0.12744400
N	4.59745700	-0.04880900	-0.04838600
C	7.83233300	2.02636300	-1.24248300
H	8.86774200	1.76483500	-0.99850900
H	7.516133	1.406932	-2.088929
H	7.819224	3.073419	-1.564246
C	7.378213	2.699864	1.15772
H	6.735318	2.562952	2.033738
H	8.405176	2.453791	1.44725
H	7.358671	3.759747	0.883185
C	-7.45192	2.497382	-1.148751
H	-8.509093	2.234917	-1.265864
H	-7.377994	3.590285	-1.132033
H	-6.912208	2.134036	-2.030171
C	-7.65408	2.418378	1.375745
H	-7.260063	1.995526	2.306006
H	-7.585151	3.509148	1.441514
H	-8.715939	2.160292	1.307178

DMAC-2Py-SO

Atoms	x	y	z
C	-2.42403000	-1.01449500	0.65233700
C	-1.32592900	-2.71828600	-0.38772500
C	-2.26358200	-2.79817800	-1.41562600
C	-3.34128000	-1.90941900	-1.38094400
C	-3.42956500	-0.99918900	-0.32833200
H	-2.46494100	-0.31368100	1.48374100
H	-2.15512700	-3.52611900	-2.21423300
H	-4.10551700	-1.91758700	-2.15295400
S	0.05060100	-3.95361000	-0.37840400
C	1.39986100	-2.73101700	-0.13978300
C	2.11348000	-2.74083600	1.05381000
C	2.64804900	-1.06342900	-1.05290700
C	3.16176900	-1.82614600	1.17017800
H	1.83817000	-3.43180900	1.84438600
C	3.43792800	-0.96915900	0.10240400
H	2.84180500	-0.41080400	-1.90142600
H	3.76110800	-1.76786700	2.07460700
C	4.19714000	1.32241300	0.53904000
C	5.74332000	-0.30815300	-0.42772500
C	5.25606800	2.23459200	0.74918100

C	2.86455900	1.75095600	0.67128600
C	6.82932600	0.57578400	-0.23485500
C	5.90412100	-1.45333100	-1.22729700
C	4.93111600	3.57021900	1.01449300
C	2.57464100	3.08210000	0.96702500
H	2.04940900	1.04925600	0.53887000
C	8.02202900	0.31186600	-0.91877100
C	7.11509300	-1.70401700	-1.87077200
H	5.08340700	-2.14901200	-1.35676900
C	3.60789500	4.00502600	1.12184500
H	5.72582800	4.29334300	1.16155200
H	1.53720900	3.39141100	1.06500700
H	8.86397400	0.98536900	-0.80211900
C	8.17682500	-0.81096500	-1.73526700
H	7.21602200	-2.59445700	-2.48588300
C	-4.32083200	1.24916500	-0.73243000
C	-5.59660900	-0.34222300	0.61998300
C	-5.42498500	2.13010500	-0.77609700
C	-3.05302900	1.68984100	-1.15065500
C	-6.72217100	0.51201400	0.59996800
C	-5.55978800	-1.43635300	1.50166900
C	-5.19577100	3.45236300	-1.17470700
C	-2.86405800	3.00537300	-1.57189000
H	-2.20782900	1.01144200	-1.14299300
C	-7.74415400	0.27460200	1.52687000
C	-6.60797400	-1.66288200	2.39251200
H	-4.71152000	-2.11083800	1.50412900
C	-3.93258100	3.90056700	-1.56852400
H	-6.02306700	4.15309200	-1.19915100
H	-1.87531200	3.32500200	-1.89076100
H	-8.61032800	0.92686900	1.54465200
C	-7.69913000	-0.79601800	2.42301800
H	-6.55699000	-2.51302200	3.06768700
N	4.50304200	-0.01708900	0.19257700
N	-4.51671200	-0.07240800	-0.25888600
N	1.64353500	-1.93754900	-1.17887100
N	-1.38958000	-1.85760200	0.62471500
H	-3.79395800	4.93179700	-1.88109400
H	-8.51467000	-0.95442400	3.12312000
H	9.12040100	-0.98849900	-2.24373700
H	3.39338400	5.04777900	1.33880600
C	6.69164200	1.69999000	0.79789700
C	-6.82580900	1.57102200	-0.50339900
C	7.73516700	2.81299500	0.59005600
H	7.64505300	3.58041600	1.36454700
H	8.75066900	2.41461100	0.67321500

H	7.63043	3.294208	-0.388959
C	6.92617	1.083919	2.21136
H	7.9376	0.665634	2.279601
H	6.81018	1.853119	2.984353
H	6.211378	0.281509	2.419868
C	-7.837228	2.678501	-0.154938
H	-7.925051	3.397208	-0.975082
H	-8.837319	2.25986	-0.008616
H	-7.55236	3.22161	0.753262
C	-7.321145	0.863705	-1.802104
H	-8.313434	0.425834	-1.640376
H	-7.384217	1.584475	-2.626202
H	-6.64012	0.06117	-2.102969
O	-0.039397	-4.748092	0.911067

DMAC-Ph-SO_2

Atoms	x	y	z
C	3.09181500	-1.18922400	-1.13893100
C	1.97949500	-2.03041600	-1.13501600
C	1.43320200	-2.42865100	0.08822500
C	1.98355600	-2.01004000	1.30092800
C	3.09690900	-1.16748900	1.28559600
C	3.65071800	-0.75277700	0.07029400
H	3.53776200	-0.87333500	-2.07763400
H	1.55412500	-2.39450900	-2.06480700
H	1.56153600	-2.35726100	2.23857400
H	3.54845400	-0.83318400	2.21491900
S	-0.00000100	-3.52877700	0.10012000
C	-1.43321500	-2.42866300	0.08824400
C	-1.97951500	-2.03041600	-1.13498900
C	-1.98356600	-2.01007100	1.30095500
C	-3.09184000	-1.18922900	-1.13888700
H	-1.55414400	-2.39449100	-2.06478600
C	-3.09692800	-1.16753200	1.28564000
H	-1.56153800	-2.35729900	2.23859600
C	-3.65074500	-0.75281100	0.07034600
H	-3.53778600	-0.87332000	-2.07758400
H	-3.54847100	-0.83324400	2.21497100
O	-0.00000700	-4.25903600	-1.17974000
O	0.00001100	-4.23120600	1.39531000
C	-6.08350600	-0.46400900	-0.09275200
C	-4.62039400	1.49387700	-0.14367100
C	-7.22335700	0.36314000	0.02735700
C	-6.23555800	-1.83093800	-0.38478100
C	-5.73443400	2.35633600	-0.02524800

C	-3.36049700	2.01874000	-0.48221800
C	-8.47799700	-0.20461300	-0.22436000
C	-7.50196000	-2.37238000	-0.60043800
H	-5.36662000	-2.47484500	-0.45265200
C	-5.55321100	3.71123100	-0.32688800
C	-3.20708700	3.37881300	-0.74704900
H	-2.49827700	1.36567800	-0.54831600
C	-8.63088200	-1.55682400	-0.53993100
H	-9.36652900	0.41346100	-0.15659500
H	-7.59585200	-3.43133400	-0.82673100
H	-6.39689900	4.38947300	-0.26153900
C	-4.30843800	4.23136800	-0.68966300
H	-2.22435300	3.76231800	-1.00944300
C	4.62042200	1.49389300	-0.14387300
C	6.08348300	-0.46402600	-0.09267900
C	5.73446200	2.35633400	-0.02541500
C	3.36056200	2.01875000	-0.48257200
C	7.22334400	0.36310600	0.02745200
C	6.23551700	-1.83098100	-0.38459500
C	5.55328100	3.71122000	-0.32714300
C	3.20719200	3.37880600	-0.74750000
H	2.49834300	1.36569200	-0.54870100
C	8.47798800	-0.20470400	-0.22412700
C	7.50192100	-2.37247700	-0.60010800
H	5.36656500	-2.47486500	-0.45249200
C	4.30855100	4.23135300	-0.69005400
H	6.39697000	4.38945700	-0.26175800
H	2.22449000	3.76230700	-1.01002000
H	9.36653400	0.41334800	-0.15635000
C	8.63086100	-1.55694700	-0.53957200
H	7.59580400	-3.43145100	-0.82631300
N	-4.79892900	0.10771800	0.08232100
N	4.79890500	0.10774500	0.08226100
H	9.62138400	-1.96521400	-0.72008600
H	4.20371400	5.29036400	-0.90891100
H	-4.20356700	5.29038800	-0.90846300
H	-9.621402	-1.96505	-0.720554
C	-7.043979	1.796044	0.540619
C	7.043959	1.796063	0.540576
C	6.908321	1.736487	2.093212
H	7.818045	1.314792	2.537267
H	6.752241	2.743242	2.499153
H	6.061311	1.112407	2.395514
C	8.25256	2.689998	0.207348
H	8.120082	3.693852	0.621649
H	9.166392	2.292647	0.658848

H	8.410066	2.778733	-0.873537
C	-6.908426	1.736329	2.093259
H	-6.752386	2.743051	2.4993
H	-7.818163	1.314581	2.537236
H	-6.061422	1.112243	2.395563
C	-8.252545	2.69002	0.207408
H	-9.166413	2.292638	0.658814
H	-8.120076	3.693833	0.621811
H	-8.409998	2.778867	-0.873477

DMAC-3Py-SO_2

Atoms	x	y	z
C	3.15240600	-1.21310200	-1.30747000
C	1.43104800	-2.40649900	-0.16257300
C	1.96021300	-1.94217800	1.04533600
C	3.60509200	-0.78149800	-0.05365400
H	3.67519000	-0.90163400	-2.20602600
H	1.52262600	-2.23848500	1.99498200
S	-0.00026900	-3.50450500	-0.16244800
C	-1.43130300	-2.40616300	-0.16142200
C	-1.96275400	-1.94635400	1.04719800
C	-3.14981200	-1.20760300	-1.30520200
H	-1.52710400	-2.24650100	1.99651900
C	-3.60510700	-0.78097700	-0.05060700
H	-3.67051700	-0.89226400	-2.20361500
O	-0.00074800	-4.20950300	-1.45529800
O	0.00005400	-4.22040300	1.12195800
C	2.03785500	-2.04537200	-1.36649900
C	-2.03552800	-2.04013500	-1.36518200
N	-3.03031100	-1.14254300	1.10159500
N	3.02770900	-1.13826300	1.09877700
H	1.65926500	-2.42410000	-2.31096600
H	-1.65516700	-2.41518800	-2.31040700
C	-6.02542000	-0.49883900	0.14256500
C	-4.55125700	1.47144500	0.00448500
C	-7.17548800	0.31661800	0.14200400
C	-6.15910700	-1.89796000	0.24902500
C	-5.65835100	2.34482300	-0.00064300
C	-3.24429300	1.99925000	-0.02143300
C	-8.42388300	-0.31600900	0.23438200
C	-7.10929600	1.84631100	0.03730600
C	-7.41382700	-2.49190300	0.33943900
H	-5.27765300	-2.52804500	0.27492700
C	-5.40235800	3.72287800	-0.04919900
C	-3.02730500	3.37254500	-0.06868400
H	-2.38981900	1.33312700	0.00950900
C	-8.56237800	-1.69970500	0.32946900

H	-9.32228300	0.29462300	0.22987500
H	-7.48648400	-3.57311800	0.42274500
H	-6.24234600	4.41152200	-0.05991300
C	-4.11227500	4.24955500	-0.08676000
H	-2.00857400	3.75123200	-0.08506100
H	-9.54952000	-2.14784300	0.39871700
H	-3.96025200	5.32451700	-0.12407500
C	4.55194400	1.47083100	-0.01233200
C	6.02452100	-0.49876300	0.15047500
C	5.65937100	2.34378800	-0.01825800
C	3.24534600	1.99888100	-0.04983600
C	7.17483400	0.31633800	0.15032600
C	6.15715700	-1.89709500	0.26793700
C	5.40419900	3.72146600	-0.07993800
C	7.10984800	1.84517000	0.03306000
C	3.02916100	3.37180300	-0.10994200
H	2.39044000	1.33333900	-0.01801600
C	8.42246300	-0.31589100	0.25501200
C	7.41113100	-2.49065800	0.37034600
H	5.27539900	-2.52676600	0.29301200
C	4.11456000	4.24825000	-0.12944200
H	6.24451500	4.40969700	-0.09154200
H	2.01069000	3.75068900	-0.13539300
H	9.32105100	0.29446900	0.25118900
C	8.55996100	-1.69884900	0.36147300
H	7.48296100	-3.57125000	0.46202400
H	3.96317400	5.32290500	-0.17682200
H	9.54653100	-2.14670700	0.44007500
N	-4.74388800	0.07647000	0.02577400
N	4.74386500	0.07603200	0.02178000
C	7.84325400	2.28559400	-1.26467700
H	8.88955	1.961376	-1.25409
H	7.362577	1.85237	-2.148692
H	7.832126	3.375768	-1.371984
C	7.820162	2.478454	1.261814
H	7.321328	2.183472	2.191089
H	8.866113	2.160069	1.321014
H	7.812318	3.571831	1.203137
C	-7.834054	2.297289	-1.261662
H	-8.880462	1.973247	-1.260542
H	-7.821978	3.388286	-1.360162
H	-7.347653	1.871027	-2.145932
C	-7.827441	2.470059	1.266373
H	-7.334791	2.167511	2.196514
H	-7.81888	3.563859	1.216448
H	-8.873864	2.151638	1.316197
C	3.15240600	-1.21310200	-1.30747000

DMAC-2Py-SO_2

Atoms	x	y	z
C	-2.94157300	-1.28915100	0.89626600
C	-1.48080300	-2.34664100	-0.48550400
C	-2.06707400	-1.83676300	-1.64380700
C	-3.16496800	-0.98998400	-1.47920800
C	-3.61345800	-0.70420100	-0.18875500
H	-3.27227700	-1.09214100	1.91366100
H	-1.68889100	-2.10676100	-2.62361200
H	-3.67504200	-0.55762200	-2.33523200
S	-0.05132400	-3.47706300	-0.65826800
C	1.41097100	-2.38007400	-0.56583900
C	2.43521900	-2.56465500	-1.49314600
C	2.51324500	-0.73040900	0.54605600
C	3.57092300	-1.76542900	-1.34910800
H	2.33740100	-3.29649300	-2.28758600
C	3.61818600	-0.83062600	-0.31318400
H	2.51578000	-0.00584700	1.35734500
H	4.41234100	-1.85708000	-2.03000200
O	-0.02103300	-4.39615500	0.48322200
O	-0.08437700	-3.98480200	-2.04569900
C	5.73213900	-0.34864400	0.83631400
C	4.73484200	1.32990300	-0.63982500
C	6.92829800	0.39926300	0.91299100
C	5.51173200	-1.41727800	1.72209600
C	5.91441600	2.10656700	-0.58741900
C	3.55617300	1.87741900	-1.17555300
C	7.83473300	0.08607900	1.93292500
C	6.44850300	-1.72297600	2.70837600
H	4.60674100	-2.00965400	1.65361700
C	5.84399600	3.43826600	-1.01315200
C	3.52689300	3.19876900	-1.61948900
H	2.65503900	1.27877800	-1.24071800
C	7.60854900	-0.95992600	2.83074800
H	8.75225600	0.65673700	2.02519800
H	6.25681700	-2.55179600	3.38469000
H	6.73064900	4.06080600	-0.96581800
C	4.66794200	3.99349500	-1.52336900
H	2.60420800	3.60258800	-2.02817900
C	-4.50594700	1.51371600	0.36789500
C	-6.01319000	-0.40964400	0.23559800
C	-5.60663300	2.39846200	0.42108700
C	-3.21428500	1.97880200	0.66955200
C	-7.13901500	0.44254300	0.28655400
C	-6.16999700	-1.79513300	0.41128600
C	-5.37461400	3.71136000	0.84783400

C	-3.01225800	3.30114100	1.06260700
H	-2.36345400	1.30996900	0.61101600
C	-8.38214600	-0.12820100	0.58429900
C	-7.42715200	-2.33638300	0.67658300
H	-5.31293600	-2.45597700	0.35257700
C	-4.09578000	4.17129500	1.17146600
H	-6.20546100	4.40502200	0.91548600
H	-2.00579800	3.63874400	1.29600800
H	-9.25933600	0.50630700	0.64767000
C	-8.53888200	-1.50215900	0.78245100
H	-7.52572200	-3.41015600	0.81239900
N	4.76706800	0.00299700	-0.14252500
N	-4.73418300	0.16076300	0.01127700
N	1.42549600	-1.49705400	0.42620600
N	-1.88869900	-2.09771900	0.75202300
H	-3.95207200	5.19951600	1.49153900
H	-9.52068500	-1.91146000	1.00345600
H	4.65302100	5.02865000	-1.85279400
H	8.33848500	-1.18003200	3.60472100
C	7.22787400	1.42687100	-0.18424200
C	-6.965895	1.916241	-0.098254
C	8.301036	2.443225	0.247157
H	9.240815	1.937503	0.487591
H	8.528672	3.137815	-0.566843
H	7.986342	3.024297	1.121366
C	7.771376	0.657621	-1.427289
H	7.974986	1.356977	-2.247049
H	8.7004	0.13383	-1.172371
H	7.049615	-0.084168	-1.783866
C	-8.126983	2.791025	0.408914
H	-8.002698	3.828507	0.084693
H	-9.079644	2.453152	-0.00956
H	-8.203535	2.775931	1.501983
C	-6.945096	2.007353	-1.65502
H	-7.894118	1.645642	-2.068563
H	-6.796101	3.046524	-1.972059
H	-6.1369	1.402826	-2.078903

DPA-Ph-SO

Atoms	x	y	z
C	-3.02868300	-1.53098800	0.44514400
C	-1.94541400	-2.27771700	-0.01205400
C	-1.37284300	-1.98173600	-1.24929800
C	-1.90536400	-0.96879400	-2.04924600
C	-2.99506100	-0.22687800	-1.59732000

C	-3.56768200	-0.49321000	-0.33931700
H	-3.46599700	-1.75226800	1.41379600
H	-1.53944700	-3.09208000	0.58191100
H	-1.49002000	-0.76439100	-3.03388600
H	-3.41607200	0.55278500	-2.22432300
S	0.02354900	-2.99010800	-1.85599700
C	1.40132800	-1.95645800	-1.24206900
C	2.06373600	-2.33659300	-0.07554100
C	1.83273700	-0.84498600	-1.96951200
C	3.13768600	-1.57887500	0.38846200
H	1.73150400	-3.22241200	0.45896600
C	2.91241600	-0.09286200	-1.51217000
H	1.34398400	-0.56707000	-2.90094200
C	3.57603300	-0.44593900	-0.32155200
H	3.64517800	-1.86657500	1.30404500
H	3.25423800	0.76531000	-2.08235000
C	5.79760500	-0.32403900	0.73767100
C	4.66157800	1.73802700	0.01930300
C	6.37330900	0.19254100	1.90974100
C	6.34923200	-1.47752200	0.15650000
C	5.80780600	2.42332300	-0.41582000
C	3.50740800	2.47275300	0.33807200
C	7.48289800	-0.43087400	2.48240400
C	7.44811100	-2.10494600	0.74481300
H	5.91328500	-1.87921000	-0.75350000
C	5.79797200	3.81475000	-0.52299500
C	3.50047500	3.86248800	0.21228200
H	2.62026400	1.95058900	0.68430200
C	8.02453800	-1.58477600	1.90783300
H	7.91663600	-0.01812500	3.38988300
H	7.86202500	-2.99778500	0.28285300
H	6.69407100	4.32923000	-0.86112800
C	4.64488400	4.54320900	-0.21493200
H	2.59911100	4.41582800	0.46435400
H	8.88404600	-2.07209000	2.35996700
H	4.63857500	5.62605000	-0.30496200
C	-4.75686100	1.65554700	-0.15132500
C	-5.71982700	-0.37328500	0.85486500
C	-5.96761200	2.22602700	-0.57685500
C	-3.63265900	2.48220100	0.01052200
C	-6.24384800	0.23237100	2.00825200
C	-6.24483400	-1.60484800	0.43073900
C	-6.05001100	3.59623800	-0.82887600
C	-3.71886400	3.84849000	-0.25972000
H	-2.69544900	2.04964400	0.34831900
C	-7.27712200	-0.38164500	2.71755500

C	-7.26622100	-2.22082700	1.15515800
H	-5.84903100	-2.07591400	-0.46423700
C	-4.92711900	4.41546100	-0.67722100
H	-6.99512800	4.02151600	-1.15732000
H	-2.83935300	4.47417200	-0.12881700
H	-7.67177200	0.10036600	3.60856500
C	-7.79156800	-1.61278500	2.29958400
H	-7.66052900	-3.17483300	0.81419400
H	-4.99289100	5.48092500	-0.88005200
H	-8.59117000	-2.09194700	2.85788100
N	4.67326700	0.31931600	0.14328300
N	-4.67415900	0.25981300	0.12121800
H	6.70310700	1.86177500	-0.66567900
H	5.94952700	1.08232200	2.36597100
H	-6.84031000	1.59267200	-0.70563300
H	-5.840104	1.183494	2.34268
O	0.039027	-4.255154	-1.011108

DPA-2Py-SO

Atoms	x	y	z
C	3.48590000	-1.28733900	1.40816700
C	1.39865800	-0.42276600	2.23597100
C	1.59439600	0.68934900	1.41179000
C	3.57990200	-0.14048200	0.58593400
H	4.26866900	-2.03683000	1.40787900
H	0.87096200	1.50212100	1.40101400
S	0.00314200	-0.54452800	3.38949000
C	-1.35525400	-0.43798800	2.18175900
C	-2.25074500	0.62668700	2.24986400
C	-2.68340900	-1.33707900	0.39425800
H	-2.10331800	1.41328200	2.98551500
C	-3.54018700	-0.21710400	0.53411600
H	-2.87073700	-2.08697400	-0.36564700
O	-0.06156000	0.73617800	4.20628500
C	-5.27658900	-1.18051800	-0.91944700
C	-5.22628800	1.24157800	-0.51526500
C	-5.53264800	-1.16608800	-2.29831400
C	-5.66157700	-2.29539900	-0.15945000
C	-6.60767800	1.42419100	-0.37626900
C	-4.42258200	2.32143200	-0.90531100
C	-6.16194300	-2.25364300	-2.90633900
C	-6.27662600	-3.38656400	-0.77598900
H	-5.48204200	-2.29989100	0.91203800
C	-7.17899500	2.67342300	-0.62796200
C	-4.99685200	3.57009000	-1.14223300
H	-3.35139700	2.18264300	-1.01258600

C	-6.53191400	-3.37060100	-2.15076000
H	-6.35604500	-2.22977300	-3.97565500
H	-6.57136000	-4.24379400	-0.17589800
H	-8.25251000	2.80271000	-0.51553600
C	-6.37728900	3.75258200	-1.00831300
H	-4.36303200	4.40155500	-1.43995100
H	-7.01826700	-4.21759700	-2.62711000
H	-6.82190200	4.72592100	-1.19794400
C	5.46247800	-1.05540100	-0.70459700
C	5.01301700	1.35803800	-0.74834600
C	6.85323700	-1.02474400	-0.53209300
C	4.86830200	-2.16161900	-1.32940200
C	5.24339300	1.55646200	-2.11509300
C	5.16806800	2.42877600	0.14221900
C	7.63782900	-2.09050000	-0.97671200
C	5.65643300	-3.23089600	-1.75900200
H	3.79230900	-2.17663700	-1.47935000
C	5.62717800	2.81396700	-2.58606400
C	5.53922500	3.68544900	-0.33565900
H	4.98896400	2.27765500	1.20193000
C	7.04385200	-3.19956200	-1.58672700
H	8.71541100	-2.05579700	-0.83855700
H	5.18560600	-4.08280300	-2.24305100
H	5.80293400	2.95600300	-3.64938600
C	5.77338700	3.88449100	-1.70031200
H	5.65262400	4.51012500	0.36334400
H	7.65626800	-4.02955800	-1.92856100
H	6.06687000	4.86407500	-2.06810900
N	-4.65393700	-0.05452100	-0.29704100
N	4.66387600	0.05068200	-0.27126100
C	2.38189500	-1.41809100	2.23875400
C	-1.59019200	-1.44545900	1.23724800
N	-3.31724900	0.73856500	1.44815100
N	2.64334300	0.82793100	0.60306200
H	-7.23060600	0.58826500	-0.07160200
H	-5.24208900	-0.29908100	-2.88444800
H	7.31191800	-0.16301900	-0.05592300
H	5.12289300	0.72627600	-2.80500900
H	2.29354400	-2.28011300	2.89668200
H	-0.91397500	-2.29236800	1.14088500

DPA-3Py-SO

Atoms	x	y	z
C	3.48590000	-1.28733900	1.40816700
C	1.39865800	-0.42276600	2.23597100
C	1.59439600	0.68934900	1.41179000
C	3.57990200	-0.14048200	0.58593400

H	4.26866900	-2.03683000	1.40787900
H	0.87096200	1.50212100	1.40101400
S	0.00314200	-0.54452800	3.38949000
C	-1.35525400	-0.43798800	2.18175900
C	-2.25074500	0.62668700	2.24986400
C	-2.68340900	-1.33707900	0.39425800
H	-2.10331800	1.41328200	2.98551500
C	-3.54018700	-0.21710400	0.53411600
H	-2.87073700	-2.08697400	-0.36564700
O	-0.06156000	0.73617800	4.20628500
C	-5.27658900	-1.18051800	-0.91944700
C	-5.22628800	1.24157800	-0.51526500
C	-5.53264800	-1.16608800	-2.29831400
C	-5.66157700	-2.29539900	-0.15945000
C	-6.60767800	1.42419100	-0.37626900
C	-4.42258200	2.32143200	-0.90531100
C	-6.16194300	-2.25364300	-2.90633900
C	-6.27662600	-3.38656400	-0.77598900
H	-5.48204200	-2.29989100	0.91203800
C	-7.17899500	2.67342300	-0.62796200
C	-4.99685200	3.57009000	-1.14223300
H	-3.35139700	2.18264300	-1.01258600
C	-6.53191400	-3.37060100	-2.15076000
H	-6.35604500	-2.22977300	-3.97565500
H	-6.57136000	-4.24379400	-0.17589800
H	-8.25251000	2.80271000	-0.51553600
C	-6.37728900	3.75258200	-1.00831300
H	-4.36303200	4.40155500	-1.43995100
H	-7.01826700	-4.21759700	-2.62711000
H	-6.82190200	4.72592100	-1.19794400
C	5.46247800	-1.05540100	-0.70459700
C	5.01301700	1.35803800	-0.74834600
C	6.85323700	-1.02474400	-0.53209300
C	4.86830200	-2.16161900	-1.32940200
C	5.24339300	1.55646200	-2.11509300
C	5.16806800	2.42877600	0.14221900
C	7.63782900	-2.09050000	-0.97671200
C	5.65643300	-3.23089600	-1.75900200
H	3.79230900	-2.17663700	-1.47935000
C	5.62717800	2.81396700	-2.58606400
C	5.53922500	3.68544900	-0.33565900
H	4.98896400	2.27765500	1.20193000
C	7.04385200	-3.19956200	-1.58672700
H	8.71541100	-2.05579700	-0.83855700
H	5.18560600	-4.08280300	-2.24305100
H	5.80293400	2.95600300	-3.64938600
C	5.77338700	3.88449100	-1.70031200
H	5.65262400	4.51012500	0.36334400

H	7.65626800	-4.02955800	-1.92856100
H	6.06687000	4.86407500	-2.06810900
N	-4.65393700	-0.05452100	-0.29704100
N	4.66387600	0.05068200	-0.27126100
C	2.38189500	-1.41809100	2.23875400
C	-1.59019200	-1.44545900	1.23724800
N	-3.31724900	0.73856500	1.44815100
N	2.64334300	0.82793100	0.60306200
H	-7.23060600	0.58826500	-0.07160200
H	-5.24208900	-0.29908100	-2.88444800
H	7.31191800	-0.16301900	-0.05592300
H	5.12289300	0.72627600	-2.80500900
H	2.29354400	-2.28011300	2.89668200
H	-0.91397500	-2.29236800	1.14088500

DPA-2Py-SO

Atoms	x	y	z
C	-3.13800600	-1.08355400	-1.58248600
C	-2.03549200	-1.89672100	-1.82958000
C	-1.28432800	-2.31126600	-0.73353200
C	-2.60077100	-1.20251300	0.76058600
C	-3.44167400	-0.71486200	-0.26066100
H	-3.75943800	-0.73225000	-2.40077000
H	-1.75253400	-2.21276000	-2.82876600
H	-2.79775000	-0.94783400	1.79875900
S	0.14017500	-3.43110600	-0.99362200
C	1.45278300	-2.21650300	-0.56404200
C	2.47035800	-2.62867400	0.29621100
C	3.50836200	-1.74028600	0.56785800
H	2.44624000	-3.61381100	0.75339300
C	2.42186400	-0.17591300	-0.90098100
C	3.50182800	-0.47393500	-0.03851600
H	4.31355200	-2.02080800	1.23965100
H	2.37288900	0.79054900	-1.39629600
O	0.20299800	-3.69567100	-2.49016500
C	5.86878900	0.03448500	0.39390000
C	4.22027200	1.86031700	0.25734900
C	6.63086500	0.56417300	1.44658600
C	6.44695400	-0.91649700	-0.46189500
C	5.03113800	2.79156000	-0.40975500
C	3.11925200	2.31573500	0.99974500
C	7.95077500	0.15060400	1.63448600
C	7.76170100	-1.33731700	-0.25712600
H	5.86571700	-1.32055500	-1.28583300
C	4.74445900	4.15503900	-0.33070400
C	2.82890300	3.67960800	1.05927600
H	2.49464500	1.60077900	1.52764900

C	8.52216500	-0.80480700	0.78870300
H	8.52952400	0.57004400	2.45355400
H	8.19626100	-2.07393400	-0.92810400
H	5.38088000	4.86490400	-0.85297200
C	3.64037300	4.60699200	0.39868800
H	1.97225500	4.01747200	1.63697800
H	9.54790500	-1.12913400	0.94112800
H	3.41589900	5.66872900	0.45258900
C	-5.33162600	-0.14349400	1.20689000
C	-4.88693900	1.19695600	-0.81396800
C	-5.72781100	0.91383800	2.04154200
C	-5.72550100	-1.45276400	1.52731600
C	-6.22816700	1.43821100	-1.15271400
C	-3.88905100	2.04027400	-1.32932000
C	-6.50684400	0.66284000	3.17180500
C	-6.48978500	-1.69742800	2.66911000
H	-5.43151800	-2.27466500	0.88092200
C	-6.56143500	2.50713800	-1.98575000
C	-4.22924000	3.09628700	-2.17589900
H	-2.84995700	1.86498600	-1.06625400
C	-6.88838700	-0.64277800	3.49601000
H	-6.80523100	1.49221100	3.80824100
H	-6.78505600	-2.71694600	2.90398700
H	-7.60452300	2.68018600	-2.23859600
C	-5.56592200	3.33964100	-2.50627100
H	-3.44442800	3.73843700	-2.56776200
H	-7.48895500	-0.83567500	4.38071600
H	-5.82806800	4.16645800	-3.16067600
N	4.52358700	0.46695300	0.19001000
N	-4.54477000	0.11245900	0.04555200
H	5.88301600	2.44251100	-0.98588100
H	6.18704700	1.29999700	2.11072800
H	-5.42451700	1.92816200	1.79949800
H	-7.00422100	0.78775500	-0.76037000
N	-1.55179800	-1.99500300	0.52981400
N	1.42504000	-1.02127500	-1.15015000

DPA-Ph-SO_2

Atoms	x	y	z
C	3.09690400	-1.41928200	-0.48333900
C	1.99197800	-2.10938100	0.00543600
C	1.43181000	-1.74544800	1.23336800
C	1.98457400	-0.69978500	1.97890900
C	3.09532500	-0.01635600	1.49473800
C	3.66669600	-0.36092100	0.25287200
H	3.52648300	-1.70128000	-1.43897900
H	1.56867200	-2.93419200	-0.55919500

H	1.56853400	-0.44903900	2.94971500
H	3.53587100	0.78003800	2.08559600
S	-0.00002900	-2.63184100	1.86060500
C	-1.43187500	-1.74542100	1.23342600
C	-1.99227200	-2.10955400	0.00565500
C	-1.98441000	-0.69954300	1.97883200
C	-3.09719800	-1.41943800	-0.48309400
H	-1.56912800	-2.93453700	-0.55884400
C	-3.09515800	-0.01609200	1.49468600
H	-1.56820900	-0.44863000	2.94952700
C	-3.66675800	-0.36085500	0.25297800
H	-3.52696400	-1.70158700	-1.43860600
H	-3.53552900	0.78047000	2.08544800
O	-0.00006100	-3.96389900	1.22509700
O	0.00001900	-2.47788700	3.32842000
C	-5.78553900	-0.34724400	-1.00518300
C	-4.96040600	1.72419500	0.02965200
C	-6.27533400	0.22259700	-2.19053500
C	-6.29429500	-1.58360600	-0.57683400
C	-6.20398700	2.21749300	0.45428700
C	-3.89157300	2.61816800	-0.14329100
C	-7.26029800	-0.43362500	-2.93055400
C	-7.26683600	-2.24175200	-1.33090000
H	-5.92537300	-2.02455700	0.34468400
C	-6.37304600	3.58147000	0.69754500
C	-4.06373900	3.97818400	0.11777100
H	-2.93003400	2.24304700	-0.48166300
C	-7.75799100	-1.67030600	-2.50897700
H	-7.63050700	0.01998500	-3.84653000
H	-7.65063500	-3.19895800	-0.98716500
H	-7.34212300	3.94843200	1.02618300
C	-5.30470500	4.46879000	0.53606100
H	-3.22679300	4.65816900	-0.02042300
H	-8.52012300	-2.18201600	-3.09032400
H	-5.43763100	5.52923400	0.73213400
C	4.96058100	1.72400400	0.02986600
C	5.78535800	-0.34731000	-1.00550100
C	6.20422800	2.21701500	0.45464400
C	3.89187800	2.61818300	-0.14283400
C	6.27522500	0.22273400	-2.19071800
C	6.29395100	-1.58385600	-0.57745600
C	6.37347700	3.58090200	0.69827600
C	4.06423000	3.97810400	0.11859900
H	2.93028200	2.24328800	-0.48129900
C	7.26009600	-0.43344100	-2.93091400
C	7.26637900	-2.24194200	-1.33169200
H	5.92498200	-2.02498300	0.34395900
C	5.30526400	4.46842000	0.53702500

H	7.34261100	3.94763600	1.02700200
H	3.22737400	4.65823700	-0.01941100
H	7.63034800	0.02036400	-3.84677600
C	7.75761400	-1.67027800	-2.50964200
H	7.65006000	-3.19928700	-0.98821200
H	5.43834600	5.52879000	0.73339100
H	8.51966900	-2.18198300	-3.09109400
N	-4.79198200	0.33296400	-0.23814100
N	4.79191900	0.33288000	-0.23829600
H	-7.03356100	1.52976600	0.58946200
H	-5.884211	1.179039	-2.52499
H	7.033717	1.529146	0.589612
H	5.884225	1.179309	-2.524933

DPA-3Py-SO_2

Atoms	x	y	z
C	-3.08732500	1.72868100	0.05158100
C	-1.41778300	1.27046100	1.71281200
C	-2.02786800	0.03177000	1.91960600
C	-3.61992900	0.43921800	0.30340400
H	-3.55604400	2.39141700	-0.66628000
H	-1.64666600	-0.65174700	2.67426200
S	0.01797300	1.75348900	2.66805000
C	1.43867200	1.16635200	1.74967300
C	1.94845000	-0.11536000	1.96626600
C	3.16810900	1.49499300	0.11910800
H	1.49836200	-0.77004800	2.70843900
C	3.61971900	0.18223400	0.40664900
H	3.66789600	2.10335100	-0.62527700
O	0.07205100	3.22821100	2.64526800
O	-0.02613500	0.99762200	3.93251600
C	5.68857000	0.47261800	-0.89133300
C	4.93189300	-1.78412900	-0.28853200
C	6.02171800	0.25753000	-2.23558900
C	6.33500300	1.48808500	-0.17201000
C	6.18256400	-2.30325100	0.06618400
C	3.91749100	-2.65136200	-0.71485200
C	6.98798200	1.05385000	-2.85306100
C	7.29005300	2.29067600	-0.79899700
H	6.08924300	1.64268900	0.87496600
C	6.41619900	-3.67828200	-0.00571700
C	4.15261300	-4.02493500	-0.77299300
H	2.94732400	-2.24966100	-0.98969900
C	7.62206200	2.07607200	-2.14027500
H	7.24004700	0.87817500	-3.89569100
H	7.78515700	3.07514100	-0.23246100
H	7.39077700	-4.07046300	0.27350100

C	5.40266500	-4.54517600	-0.42173900
H	3.35756100	-4.68988100	-1.10064700
H	8.37115400	2.69706200	-2.62402700
H	5.58362100	-5.61554100	-0.47207500
C	-5.11243900	0.53661600	-1.64833800
C	-5.53410100	-1.10373400	0.12947500
C	-6.41765800	1.01038800	-1.83892700
C	-4.19497000	0.59213200	-2.70746800
C	-5.84959400	-2.18946000	-0.69581900
C	-6.03825400	-1.05637400	1.43575300
C	-6.79735800	1.53756300	-3.07459700
C	-4.57627500	1.13360100	-3.93657700
H	-3.18874700	0.20802800	-2.56441700
C	-6.66368500	-3.21895700	-0.21827300
C	-6.84076900	-2.09330100	1.91124200
H	-5.79360100	-0.21533300	2.07667000
C	-5.87851900	1.60634900	-4.12626800
H	-7.81214500	1.90187600	-3.21198600
H	-3.85748600	1.17182100	-4.75114000
H	-6.90195500	-4.05754000	-0.86761400
C	-7.15972200	-3.17767600	1.08712300
H	-7.22365700	-2.04926900	2.92758800
H	-6.17534800	2.02075400	-5.08591900
H	-7.78895800	-3.98151900	1.45977800
N	4.71655300	-0.36517800	-0.25462400
N	-4.73509300	-0.02857300	-0.38764800
C	-1.97345500	2.13858100	0.76317300
C	2.07005600	1.98529200	0.80400700
N	3.00897200	-0.59726100	1.31763500
N	-3.09365900	-0.37975500	1.23206800
H	6.96828300	-1.63027200	0.39682800
H	5.52637800	-0.53659600	-2.78678500
H	-7.12858600	0.95771500	-1.01948100
H	-5.45874900	-2.22451300	-1.70860200
H	-1.55477300	3.12999600	0.61878000
H	1.703904	2.990839	0.620056

DPA-2Py-SO_2

Atoms	x	y	z
C	2.80812700	-0.00431400	-1.29041100
C	1.50333000	-1.82021800	-0.84633300
C	2.27906100	-2.20470900	0.24872800
C	3.38306200	-1.42025300	0.56914000
C	3.67423500	-0.28480700	-0.20763100
H	2.98850100	0.85906300	-1.92508400
H	2.02344500	-3.08940900	0.82116400
H	4.01595800	-1.68322000	1.41069100

S	0.08472500	-2.85306400	-1.33038200
C	-1.38849000	-1.93348000	-0.78193500
C	-2.15271000	-2.44089100	0.26991800
C	-2.76541100	-0.14131500	-1.08134200
C	-3.29865700	-1.74070400	0.63616000
H	-1.86641300	-3.36350400	0.76230700
C	-3.63501000	-0.55847000	-0.04654600
H	-2.97365000	0.76995600	-1.63547900
H	-3.93188400	-2.10799800	1.43740900
O	0.05511000	-2.97569600	-2.79191900
O	0.14827500	-4.05400000	-0.46643900
C	-5.50126700	0.88807800	-0.74028800
C	-5.27241600	0.21784800	1.61715900
C	-5.91781400	2.20981500	-0.52176700
C	-5.81305800	0.25984000	-1.95580900
C	-6.63570600	0.00916000	1.87515000
C	-4.40121300	0.47068000	2.68834100
C	-6.63718800	2.88963600	-1.50581800
C	-6.51730000	0.95227700	-2.94196900
H	-5.50192700	-0.76682100	-2.12636700
C	-7.11699200	0.05593400	3.18463100
C	-4.88689900	0.49940400	3.99639300
H	-3.34725400	0.64588500	2.49193200
C	-6.93618200	2.26795600	-2.72197900
H	-6.95358700	3.91362000	-1.32413200
H	-6.74845600	0.45492000	-3.88034700
H	-8.17556400	-0.10738600	3.37001300
C	-6.24657100	0.29577100	4.25207100
H	-4.20089200	0.69624700	4.81638600
H	-7.48945800	2.80229400	-3.48937400
H	-6.62318600	0.32557300	5.27081000
C	4.72246800	1.94217800	-0.18664300
C	5.97496000	-0.01756600	0.61959700
C	5.78578500	2.58419900	-0.83903300
C	3.61406300	2.69650600	0.22825500
C	6.59849400	0.60060200	1.71387500
C	6.54379400	-1.17578300	0.06740300
C	5.73856000	3.95981200	-1.06989300
C	3.56634400	4.06873900	-0.02177700
H	2.79299500	2.20587600	0.74319600
C	7.77494700	0.06758200	2.24355300
C	7.71095800	-1.71227600	0.61304600
H	6.07161800	-1.65031600	-0.78809700
C	4.62827100	4.70860900	-0.66812100
H	6.56854000	4.44427900	-1.57783200
H	2.70004400	4.64015600	0.30164300
H	8.24844000	0.55690200	3.09093400
C	8.33455000	-1.09296400	1.70077500

H	8.14077900	-2.60969200	0.17551400
H	4.59091400	5.77803800	-0.85641000
H	9.24711300	-1.50897200	2.11880200
N	-4.78080300	0.18744900	0.27648400
N	4.78005800	0.53701800	0.06592900
N	-1.67777400	-0.81650000	-1.44216900
N	1.75242600	-0.75262200	-1.59784800
H	6.16100700	1.49784600	2.14186200
H	6.64435800	2.00267800	-1.16171400
H	-7.31257900	-0.18573300	1.04853800
H	-5.677657	2.697649	0.418439