Exploring the Role of Squaraine infusion on Two-Photon Absorption Cross-Section of a few BODIPY like Systems

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1. Oscillator strengths & Excitation energies of $S_0 \rightarrow S_1$ transition :

The table presents the oscillator strengths, excitation energies (in eV), excitation wavelengths (in nm) corresponding to the $S_0 \rightarrow S_1$ transition of all the considered systems calculated at RI-CC2/cc-pVDZ level of theory as implemented in Turbomole 7.3 program.

ST1a : bdpsq fusion scheme

System	S_1-Osc. Str. (unitless)	S_1-Ex. En. (eV)	S_1-Ex. WL (nm)	System	S_1-Osc. Str. (unitless)	S_1-Ex. En. (eV)	S_1-Ex. WL (nm)
bdpsq-pristine	1.23	2.79	445.14	4-enNMe2	1.92	2.38	520.31
1-enNMe2	1.76	2.53	490.53	4-enPY5	1.74	2.36	526.43
1-enPY5	1.90	2.51	493.96	4-enPY6	1.71	2.45	506.89
1-enPY6	1.82	2.54	488.54	4-NMe2	1.54	2.52	492.36
1-NMe2	1.37	2.71	457.58	4-PY5	1.63	2.52	492.98
1-PY5	1.54	2.63	471.09	4-PY6	1.56	2.59	478.25
1-PY6	1.48	2.65	467.29	5-enNMe2	0.90	2.21	562.21
2-enNMe2	0.98	2.22	558.38	5-enPY5	1.27	2.40	516.58
2-enPY5	1.26	2.37	524.00	5-enPY6	1.55	2.58	480.25
2-enPY6	1.60	2.50	495.94	5-NMe2	0.79	2.20	563.46
2-NMe2	0.88	2.40	515.76	5-PY5	1.19	2.51	494.44
2-PY5	1.25	2.57	482.28	5-PY6	1.41	2.69	461.76
2-PY6	1.53	2.65	467.61	6-enNMe2	0.74	2.08	595.21
3-enNMe2	0.45	2.09	592.03	6-enPY5	0.81	2.23	555.21
3-enPY5	0.79	2.36	524.76	6-enPY6	1.05	2.50	496.99
3-enPY6	1.25	2.56	484.51	6-NMe2	1.01	2.51	493.10
3-NMe2	0.66	2.61	474.99	6-PY5	0.79	2.44	507.95
3-PY5	0.65	2.49	498.03	6-PY6	1.15	2.68	462.26
3-PY6	1.19	2.66	466.46				

ST1b : bdp2sq fusion scheme

System	S_1-Osc. Str. (unitless)	S_1-Ex. En. (eV)	S_1-Ex. WL (nm)	System	S_1-Osc. Str. (unitless)	S_1-Ex. En. (eV)	S_1-Ex. WL (nm)
bdp2sq-pristine	1.30	2.81	441.91	3-enNMe2	0.44	1.97	628.96
1-enNMe2	1.87	2.41	515.06	3-enPY5	0.67	2.21	560.48
1-enPY5	2.04	2.41	513.56	3-enPY6	0.79	2.48	500.77
1-enPY6	1.99	2.51	493.41	3-NMe2	0.68	2.50	495.78
1-NMe2	1.47	2.59	478.16	3-PY5	0.54	2.40	516.56
1-PY5	1.68	2.56	485.30	3-PY6	1.25	2.71	457.75
1-PY6	1.60	2.66	466.34				
2-enNMe2	0.91	2.02	613.10				
2-enPY5	1.09	2.20	563.28				
2-enPY6	1.45	2.43	509.43				
2-NMe2	0.83	2.24	554.21				
2-PY5	1.11	2.45	507.10				
2-PY6	1.54	2.65	468.22				

2. TPA strengths [RI-CC2] of $S_0 \rightarrow S_1$ transition:

The table presents the TPA strengths (in a.u. and GM units) corresponding to the $S_0 \rightarrow S_1$ transition of all the considered systems calculated at RI-CC2/cc-pVDZ level of theory as implemented in Turbomole 7.3 program.

ST2a : bdpsq fusion scheme

System	TPA-S_1 (a.u.)	TPA-S_1 (GM)	System	TPA-S_1 (a.u.)	TPA-S_1 (GM)
bdpsq-pristine	7842	162	4-enNMe2	21030	318
1-enNMe2	5753	98	4-enPY5	43673	644
1-enPY5	3835	64	4-enPY6	23494	374
1-enPY6	13150	225	4-NMe2	458	8
1-NMe2	21902	428	4-PY5	14246	240
1-PY5	10102	186	4-PY6	17407	311
1-PY6	9443	177	5-enNMe2	159270	2061
2-enNMe2	55430	727	5-enPY5	118632	1818
2-enPY5	32324	481	5-enPY6	49134	871
2-enPY6	38	1	5-NMe2	61226	789
2-NMe2	2706	42	5-PY5	41120	688
2-PY5	113	2	5-PY6	23120	443
2-PY6	5393	101	6-enNMe2	28322	327
3-enNMe2	13628	159	6-enPY5	54577	724
3-enPY5	29065	432	6-enPY6	14170	235
3-enPY6	5564	97	6-NMe2	1142	19
3-NMe2	2052	37	6-PY5	10006	159
3-PY5	5033	83	6-PY6	6889	132
3-PY6	8803	165			

ST2b : bdp2sq fusion scheme

System	TPA-S_1 (a.u.)	TPA-S_1 (GM)	System	TPA-S_1 (a.u.)	TPA-S_1 (GM)
bdp2sq-pristine	0	0	3-enNMe2	17360	179
1-enNMe2	2494	38	3-enPY5	58422	761
1-enPY5	17717	275	3-enPY6	4485	73
1-enPY6	868	15	3-NMe2	1297	22
1-NMe2	8877	159	3-PY5	8044	123
1-PY5	589	10	3-PY6	15	0
1-PY6	173	3			
2-enNMe2	135126	1470			
2-enPY5	122157	1574			
2-enPY6	25312	399			
2-NMe2	18134	241			
2-PY5	20992	334			
2-PY6	2678	50			

3. 2SM data of $S_0 \rightarrow S_1$ transition:

ST3a : The table presents the TPA strengths (in a.u.) of S_1 state evaluated employing 2SM for top 2 TP active systems from each fusion scheme (based on TPA [RI-CC2] strengths) and their respective non-conjugated counterparts.

System	TPA-S_1 (2SM) in a.u.	**System**	TPA-S_1 (2SM) in a.u.
bdpsq-5-enNMe2	200100	bdp2sq-2-enNMe2	130800
bdpsq-5-NMe2	61240	bdp2sq-2-NMe2	18940
bdpsq-5-enPY5	147900	bdp2sq-2-enPY5	140500
bdpsq-5-PY5	45590	bdp2sq-2-PY5	31370

ST3b : Cosine values of angle between transition dipole moments involved in δ_{01kl} for top 2 TP active systems from each fusion scheme (based on TPA [RI-CC2] strengths) and their respective non-conjugated counterparts, which are evaluated at RI-CC2/cc-pVDZ level of theory.

System	Cosθ (00-10)	Cosθ (01-00)	Cosθ (01-10)	Cosθ (11-01)	Cosθ (11-00)	Cosθ (10-11)
bdpsq-5-enNMe2	-0.928	-0.923	1	-0.999	0.941	-0.999
bdpsq-5-NMe2	0.907	0.902	1	0.996	0.935	0.997
bdpsq-5-enPY5	0.898	0.892	1	0.992	0.942	0.994
bdpsq-5-PY5	0.955	0.952	1	0.998	0.967	0.999
bdp2sq-2-enNMe2	0.972	0.975	1	0.973	1	0.970
bdp2sq-2-NMe2	0.989	0.991	1	0.966	0.990	0.962
bdp2sq-2-enPY5	0.908	0.912	1	0.957	0.992	0.954
bdp2sq-2-PY5	0.904	0.907	1	0.944	0.995	0.941

4. Ground state dipole moments of the fused systems with substitutions:

The following tables presents the ground state dipole moment strengths (in Debye) of all the considered systems calculated at B3LYP/6-311+g(d,p) level of theory as implemented in Gaussian 16 program.

ST4a : Dipole moment strengths of bdpsq fusion scheme.

System	Dipole Moment (Debye)	System	Dipole Moment (Debye)
bdpsq-1-enNMe2	5.73	bdpsq-1-NMe2	3.70
bdpsq-1-enPY5	4.38	bdpsq-1-PY5	3.31
bdpsq-1-enPY6	5.87	bdpsq-1-PY6	6.67
bdpsq-2-enNMe2	6.12	bdpsq-2-NMe2	4.23
bdpsq-2-enPY5	6.21	bdpsq-2-PY5	5.40
bdpsq-2-enPY6	6.71	bdpsq-2-PY6	6.74
bdpsq-3-enNMe2	9.47	bdpsq-3-NMe2	7.15
bdpsq-3-enPY5	8.65	bdpsq-3-PY5	7.50
bdpsq-3-enPY6	3.60	bdpsq-3-PY6	4.11
bdpsq-4-enNMe2	13.45	bdpsq-4-NMe2	10.98
bdpsq-4-enPY5	11.21	bdpsq-4-PY5	10.38

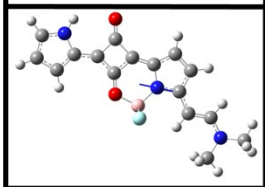
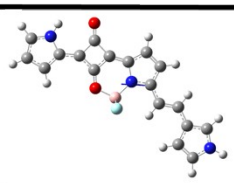
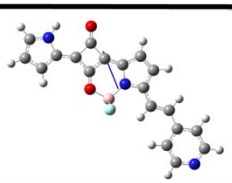
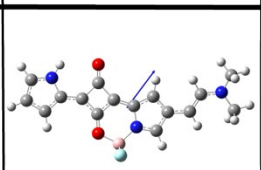
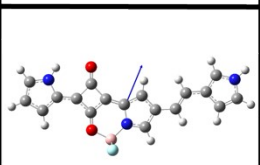
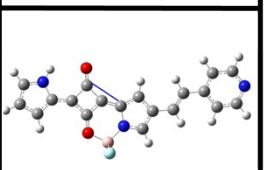
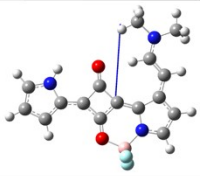
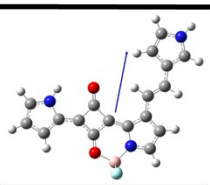
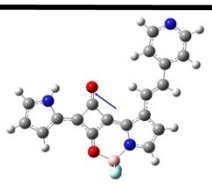
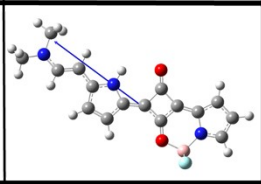
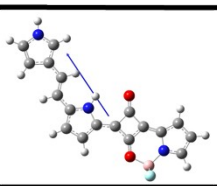
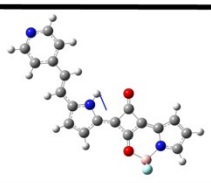
bdpsq-4-enPY6	2.70	bdpsq-4-PY6	2.52
bdpsq-5-enNMe2	8.28	bdpsq-5-NMe2	6.59
bdpsq-5-enPY5	8.32	bdpsq-5-PY5	5.76
bdpsq-5-enPY6	5.18	bdpsq-5-PY6	5.11
bdpsq-6-enNMe2	6.96	bdpsq-6-NMe2	6.92
bdpsq-6-enPY5	5.72	bdpsq-6-PY5	3.73
bdpsq-6-enPY6	6.78	bdpsq-6-PY6	6.44

ST4b : Dipole moment strengths of bdp2sq fusion scheme.

System	Dipole Moment (Debye)	System	Dipole Moment (Debye)
bdp2sq-1-enNMe2	10.83	bdp2sq-1-NMe2	7.62
bdp2sq-1-enPY5	9.14	bdp2sq-1-PY5	7.11
bdp2sq-1-enPY6	0.91	bdp2sq-1-PY6	1.75
bdp2sq-2-enNMe2	6.76	bdp2sq-2-NMe2	4.58
bdp2sq-2-enPY5	5.57	bdp2sq-2-PY5	4.41
bdp2sq-2-enPY6	2.71	bdp2sq-2-PY6	2.82
bdp2sq-3-enNMe2	6.66	bdp2sq-3-NMe2	5.22
bdp2sq-3-enPY5	6.60	bdp2sq-3-PY5	3.81
bdp2sq-3-enPY6	1.66	bdp2sq-3-PY6	2.14

The following figures illustrate the ground state dipole moment vector orientations of all the considered systems calculated at B3LYP/6-311+g(d,p) level of theory as implemented in Gaussian 16 program.

SF4a : Dipole moment vectors of systems with bdpsq fusion scheme

1-enNMe2	1-enPY5	1-enPY6	2-enNMe2	2-enPY5	2-enPY6
					
3-enNMe2	3-enPY5	3-enPY6	4-enNMe2	4-enPY5	4-enPY6
					
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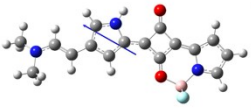		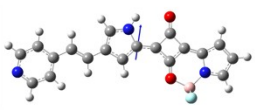	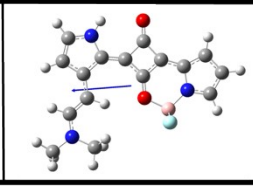	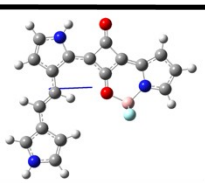	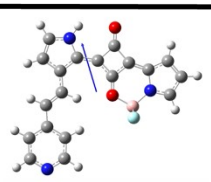

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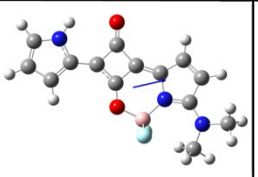	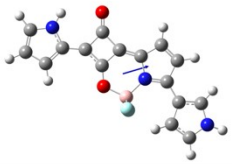	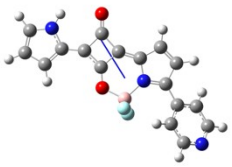		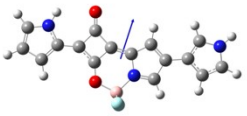	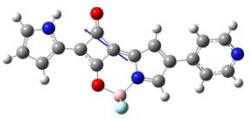
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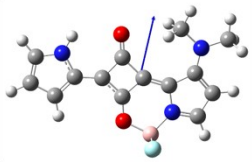
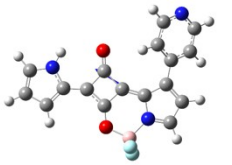
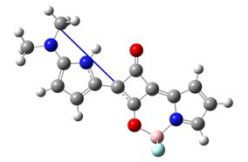
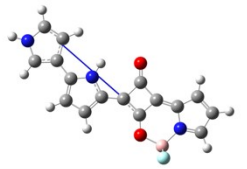
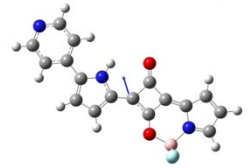
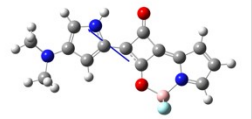
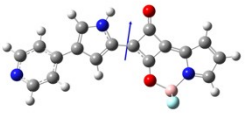
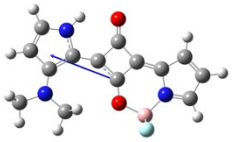
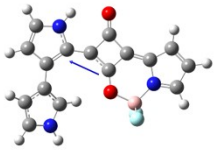
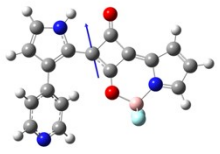
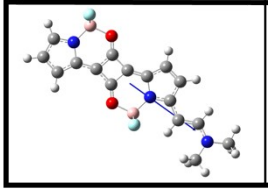
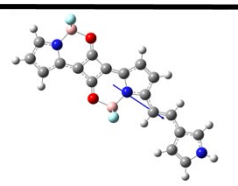
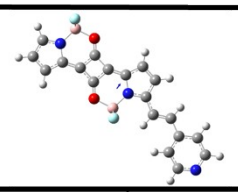
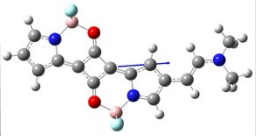
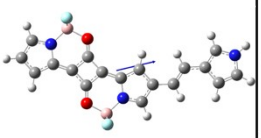
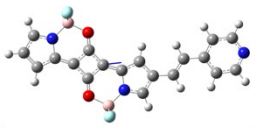
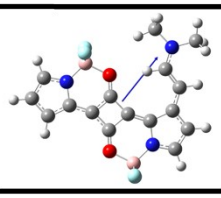
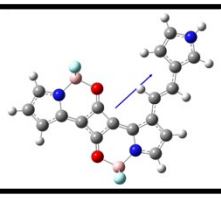
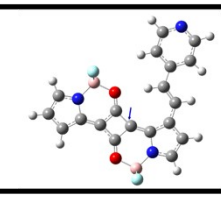
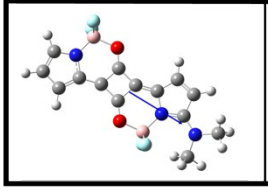
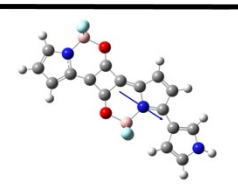
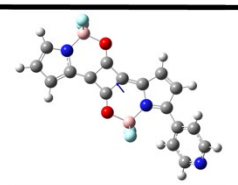
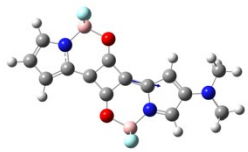
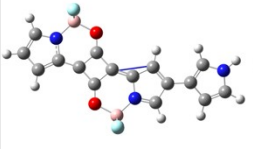
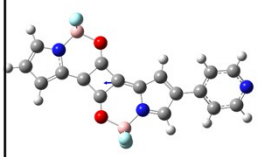
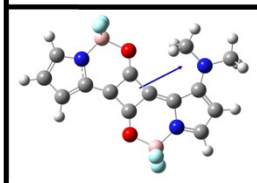
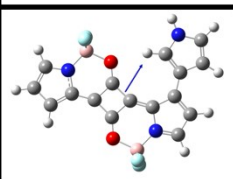
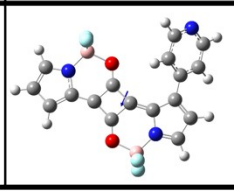
					
5-NMe2	5-PY5	5-PY6	6-NMe2	6-PY5	6-PY6
					

SF4b : Dipole moment vectors of systems with bdp2sq fusion scheme

1-enNMe2	1-enPY5	1-enPY6	2-enNMe2	2-enPY5	2-enPY6
					

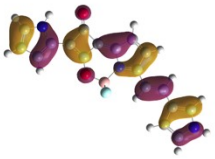
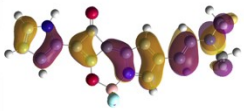
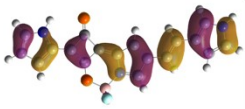
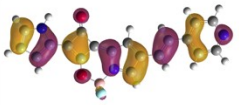
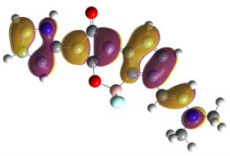
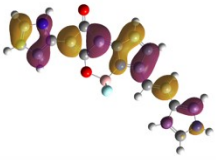
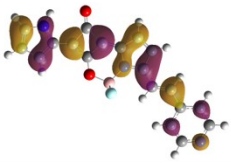
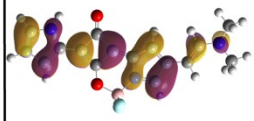
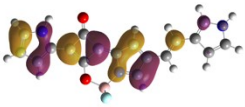
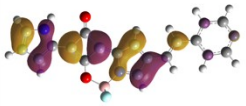
3-enNMe2	3-enPY5	3-enPY6
		

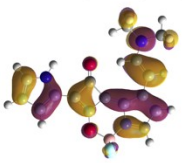
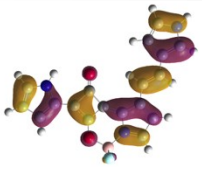
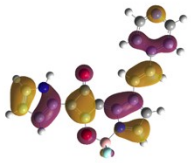
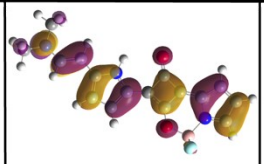
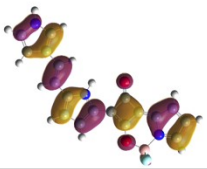
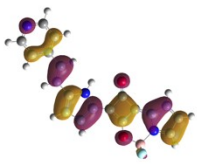
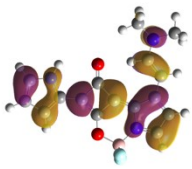
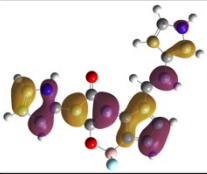
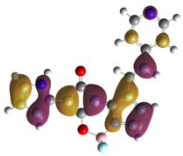
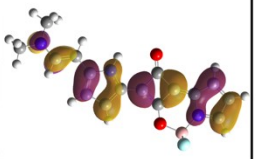
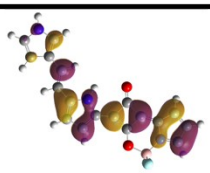
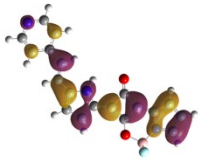
1-NMe2	1-PY5	1-PY6	2-NMe2	2-PY5	2-PY6
					

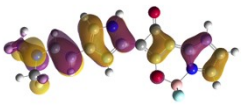
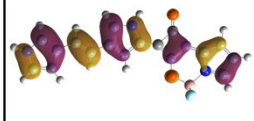
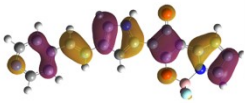
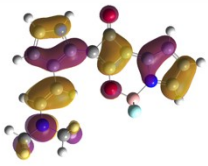
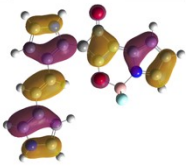
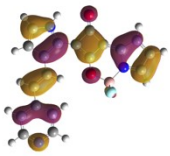
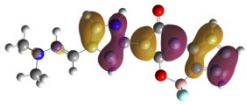
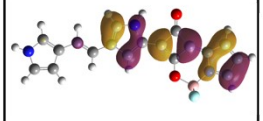
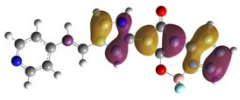
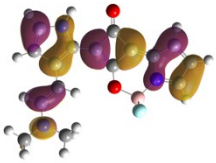
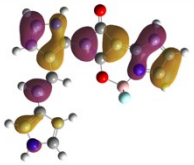
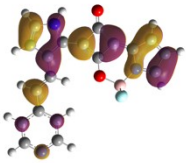
3-NMe2	3-PY5	3-PY6
		

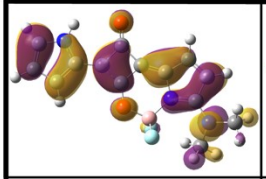
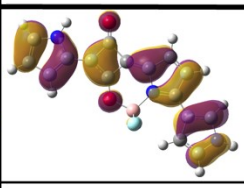
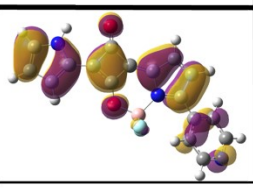
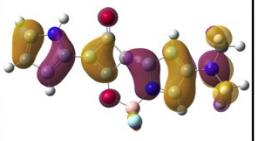
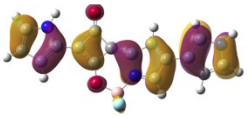
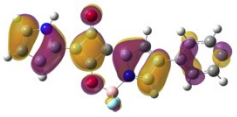
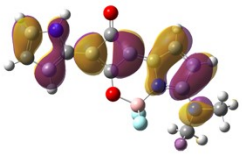
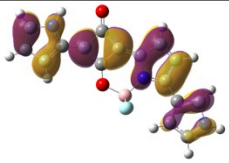
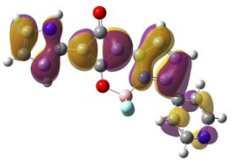
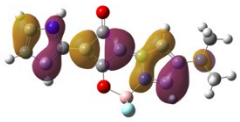
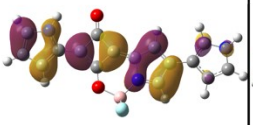
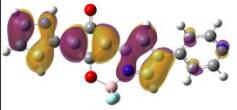
5. MOs involved in $S_0 \rightarrow S_1$ transition :

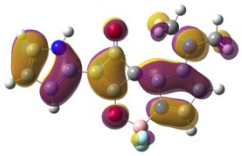
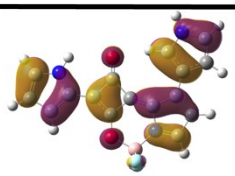
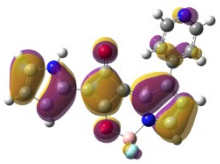
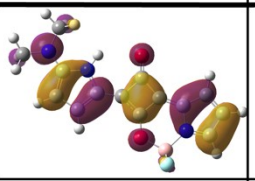
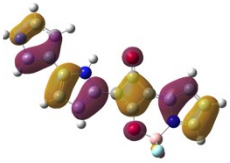
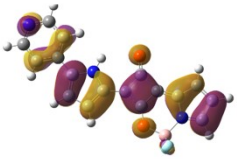
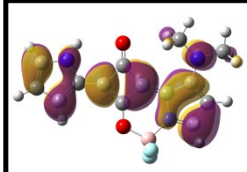
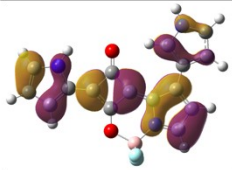
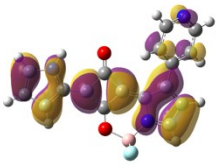
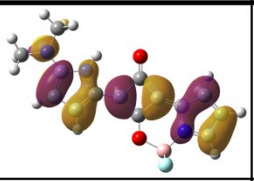
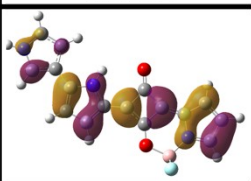
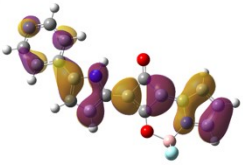
The following figures presents the MOs involved in $S_0 \rightarrow S_1$ transition for all the considered systems.
SF5a : MOs corresponding to $S_0 \rightarrow S_1$ transition of systems with bdpsq fusion scheme

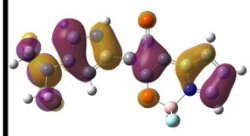
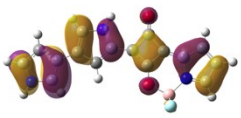
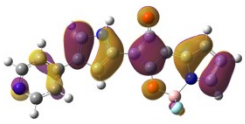
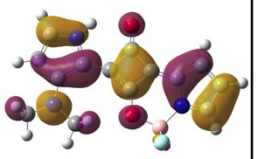
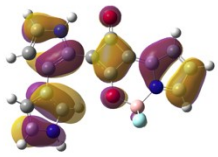
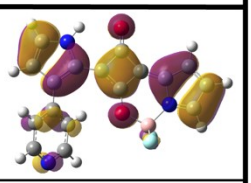
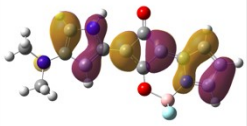
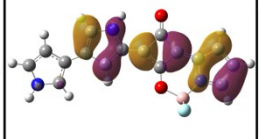
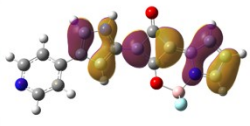
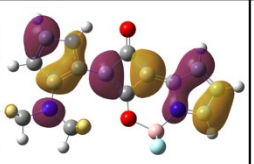
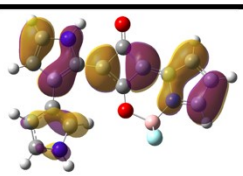
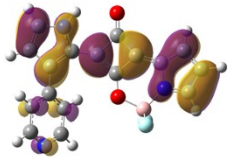
1-enNMe2	1-enPY5	1-enPY6	2-enNMe2	2-enPY5	2-enPY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

3-enNMe2	3-enPY5	3-enPY6	4-enNMe2	4-enPY5	4-enPY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

5-enNMe2	5-enPY5	5-enPY6	6-enNMe2	6-enPY5	6-enPY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

1-NMe2	1-PY5	1-PY6	2-NMe2	2-PY5	2-PY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

3-NMe2	3-PY5	3-PY6	4-NMe2	4-PY5	4-PY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

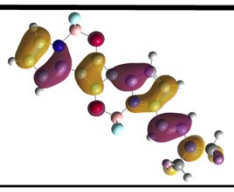
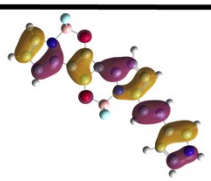
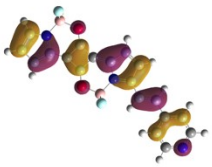
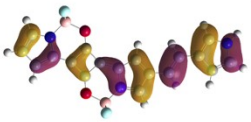
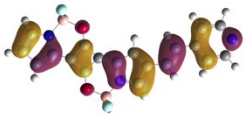
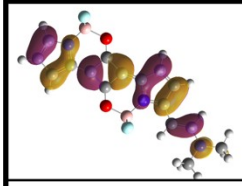
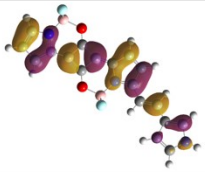
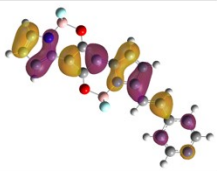
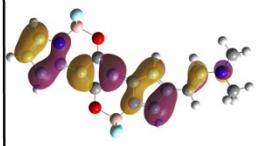
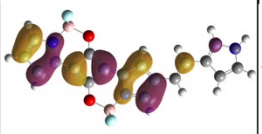
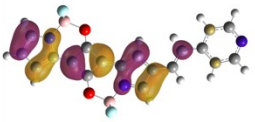
5-NMe2	5-PY5	5-PY6	6-NMe2	6-PY5	6-PY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

ST5a : MO contributions (in %) corresponding to $S_0 \rightarrow S_1$ transition of systems with bdpsq fusion scheme computed at RI-CC2/cc-pVDZ level of theory.

System	From	To	Weight (%)	System	From	To	Weight (%)
bdpsq-1-enNMe2	HOMO	LUMO	92.5	bdpsq-1-NMe2	HOMO	LUMO	93.5
bdpsq-1-enPY5	HOMO	LUMO	94.6	bdpsq-1-PY5	HOMO	LUMO	94.6
bdpsq-1-enPY6	HOMO	LUMO	94.5	bdpsq-1-PY6	HOMO	LUMO	94.2

bdpsq-2-enNMe2	HOMO	LUMO	78.6	bdpsq-2-NMe2	HOMO	LUMO	69.5
	HOMO-1	LUMO	16		HOMO-1	LUMO	21.6
bdpsq-2-enPY5	HOMO	LUMO	91.4	bdpsq-2-PY5	HOMO	LUMO	90.3
bdpsq-2-enPY6	HOMO	LUMO	92.7	bdpsq-2-PY6	HOMO	LUMO	93.6
bdpsq-3-enNMe2	HOMO	LUMO	58.9	bdpsq-3-NMe2	HOMO	LUMO	56.1
	HOMO-1	LUMO	37.7		HOMO-1	LUMO	39.2
bdpsq-3-enPY5	HOMO	LUMO	72.9	bdpsq-3-PY5	HOMO	LUMO	70.3
	HOMO-1	LUMO	19.4		HOMO-1	LUMO	21.8
bdpsq-3-enPY6	HOMO	LUMO	91.6	bdpsq-3-PY6	HOMO	LUMO	94.3
bdpsq-4-enNMe2	HOMO	LUMO	93.5	bdpsq-4-NMe2	HOMO	LUMO	93.8
bdpsq-4-enPY5	HOMO	LUMO	94.9	bdpsq-4-PY5	HOMO	LUMO	94.9
bdpsq-4-enPY6	HOMO	LUMO	94.8	bdpsq-4-PY6	HOMO	LUMO	94.5
bdpsq-5-enNMe2	HOMO	LUMO	84.5	bdpsq-5-NMe2	HOMO	LUMO	70.8
	HOMO-1	LUMO	11.8		HOMO-1	LUMO	24.4
bdpsq-5-enPY5	HOMO	LUMO	93.6	bdpsq-5-PY5	HOMO	LUMO	92.1
bdpsq-5-enPY6	HOMO	LUMO	93.7	bdpsq-5-PY6	HOMO	LUMO	93.6
bdpsq-6-enNMe2	HOMO	LUMO	78.9	bdpsq-6-NMe2	HOMO	LUMO	82.2
	HOMO-1	LUMO	17.3		HOMO-1	LUMO	12.9
bdpsq-6-enPY5	HOMO	LUMO	89.3	bdpsq-6-PY5	HOMO	LUMO	86.3
bdpsq-6-enPY6	HOMO	LUMO	93.8	bdpsq-6-PY6	HOMO	LUMO	94

SF5b : MOs corresponding to $S_0 \rightarrow S_1$ transition of systems with bdp2sq fusion scheme

1-enNMe2	1-enPY5	1-enPY6	2-enNMe2	2-enPY5	2-enPY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
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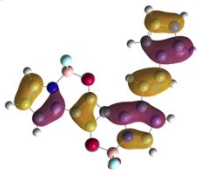
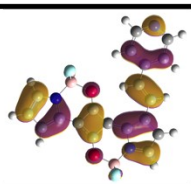
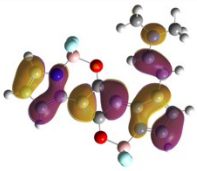
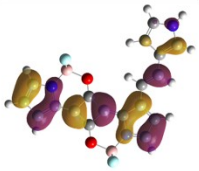
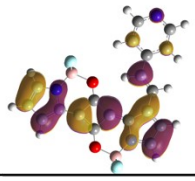
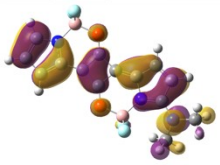
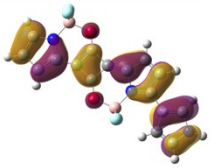
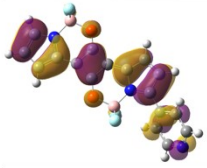
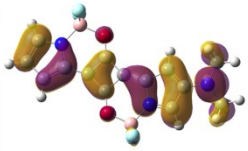
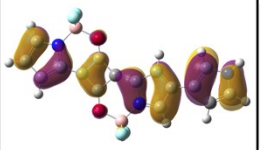
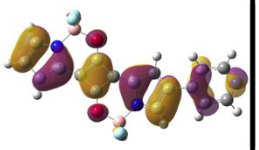
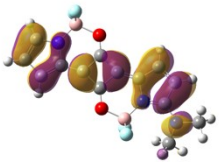
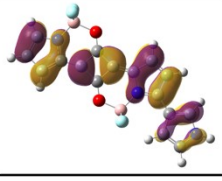
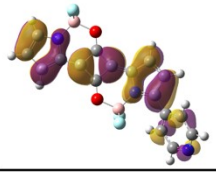
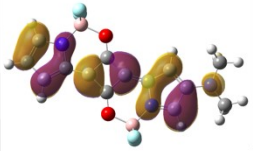
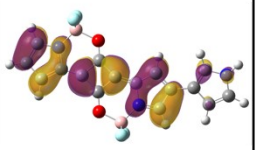
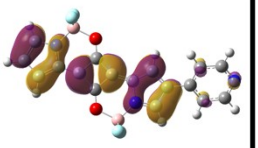
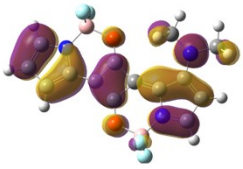
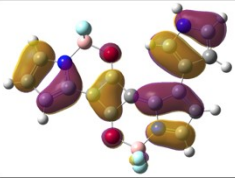
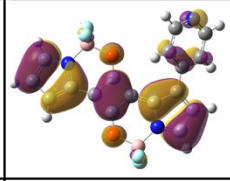
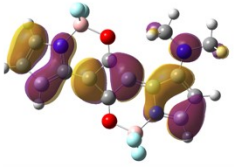
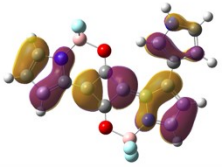
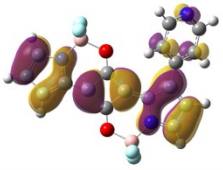
3-enNMe2	3-enPY5	3-enPY6
		
HOMO	HOMO	HOMO
		
LUMO	LUMO	LUMO

1-NMe2	1-PY5	1-PY6	2-NMe2	2-PY5	2-PY6
					
HOMO	HOMO	HOMO	HOMO	HOMO	HOMO
					
LUMO	LUMO	LUMO	LUMO	LUMO	LUMO

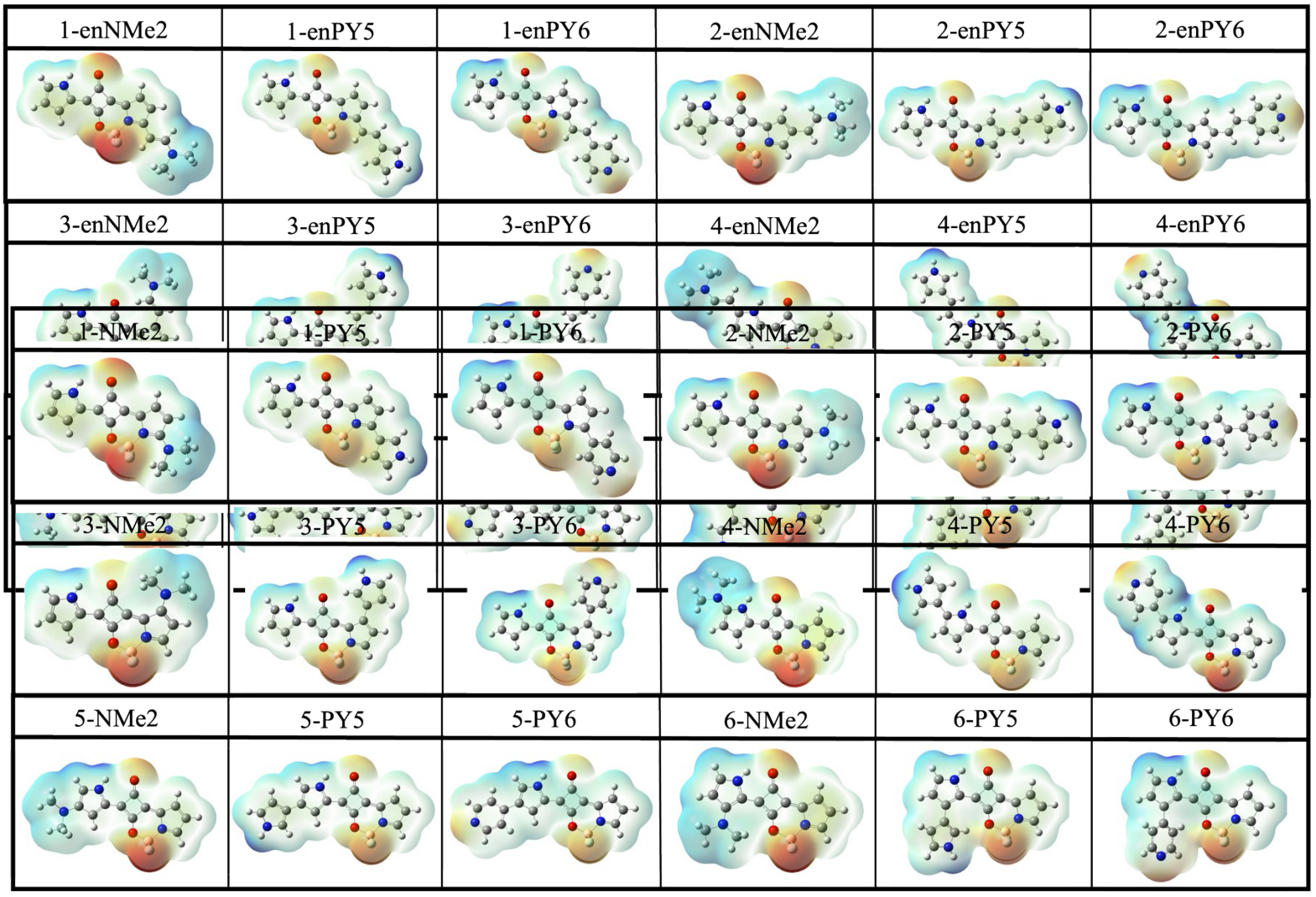
3-NMe2	3-PY5	3-PY6
		
HOMO	HOMO	HOMO
		
LUMO	LUMO	LUMO

ST5b : MO contributions (in %) corresponding to $S_0 \rightarrow S_1$ transition of systems with bdp2sq fusion scheme computed at RI-CC2/cc-pVDZ level of theory.

System	From	To	Weight (%)	System	From	To	Weight (%)
bdp2sq-1-enNMe2	HOMO	LUMO	91.2	bdp2sq-1-NMe2	HOMO	LUMO	92.4
bdp2sq-1-enPY5	HOMO	LUMO	93.8	bdp2sq-1-PY5	HOMO	LUMO	94.2
bdp2sq-1-enPY6	HOMO	LUMO	94.5	bdp2sq-1-PY6	HOMO	LUMO	94
bdp2sq-2-enNMe2	HOMO	LUMO	78.4	bdp2sq-2-NMe2	HOMO	LUMO	66.4
	HOMO-1	LUMO	16.9		HOMO-1	LUMO	25.6
bdp2sq-2-enPY5	HOMO	LUMO	90.2	bdp2sq-2-PY5	HOMO	LUMO	86.3
bdp2sq-2-enPY6	HOMO	LUMO	90.8		HOMO-1	LUMO	5.1
bdp2sq-3-enNMe2	HOMO	LUMO	62.2	bdp2sq-2-PY6	HOMO	LUMO	92.2
	HOMO-1	LUMO	34.4	bdp2sq-3-NMe2	HOMO	LUMO	59.8
bdp2sq-3-enPY5	HOMO	LUMO	72.4		HOMO-1	LUMO	35.4
	HOMO-1	LUMO	19.4	bdp2sq-3-PY5	HOMO	LUMO	64.8
bdp2sq-3-enPY6	HOMO	LUMO	81.9		HOMO-1	LUMO	25.9
	HOMO-1	LUMO	13.3	bdp2sq-3-PY6	HOMO	LUMO	94

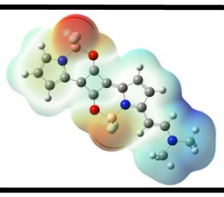
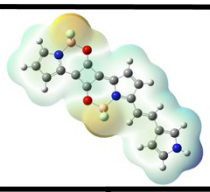
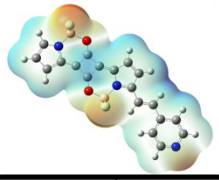
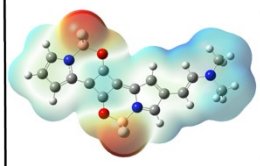
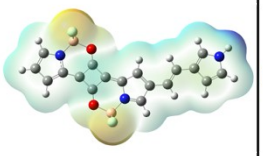
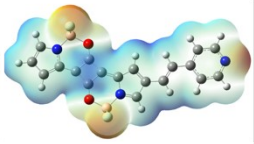
6. Electrostatic potential surfaces of the fused systems substitutions :

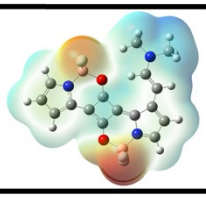
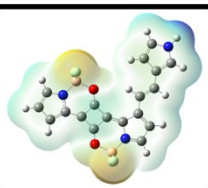
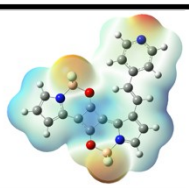
SF6a : ESPs of systems with bdpsq fusion scheme

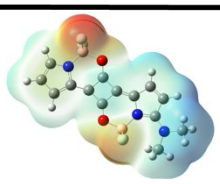
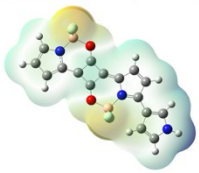
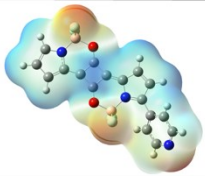
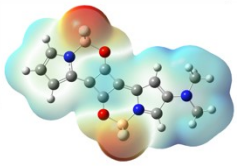
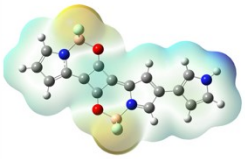
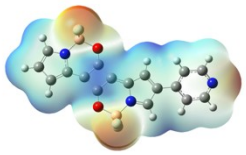


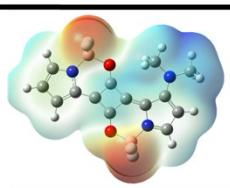
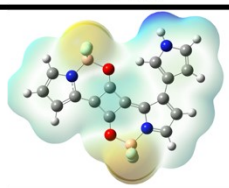
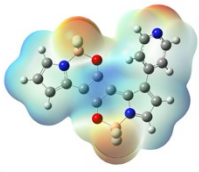
Pristine bdpsq

SF6b : ESPs of systems with bdp2sq fusion scheme

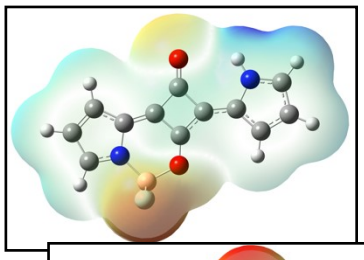
1-enNMe2	1-enPY5	1-enPY6	2-enNMe2	2-enPY5	2-enPY6
					

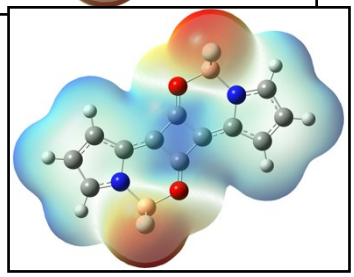
3-enNMe2	3-enPY5	3-enPY6
		

1-NMe2	1-PY5	1-PY6	2-NMe2	2-PY5	2-PY6
					

3-NMe2	3-PY5	3-PY6
		

Pristine-bdp2sq





7. Effect of cis and trans conformation on TPA strengths :

ST7 : Comparison of ground state dipole moments, S_1 excitation energies and S_1 two-photon absorption strengths between cis- and trans-conformers of the top two most TP active bdpsq systems.

System	S_0 Dipole (Debye)	S_1 Ex.Ene (eV)	S1 TPA (a.u.)
bdpsq-5-enNMe2	8.28	2.206	159269
bdpsq-5-enNMe2-cis	6.95	2.391	88217
bdpsq-5-enPY5	8.32	2.401	118631
bdpsq-5-enPY5-cis	7.50	2.482	67371

8. Optimized Coordinates of the ground-state geometry :

This section includes the vacuum phase ground-state optimized cartesian coordinates for all the systems considered in this work that are optimized at B3LYP/6-311+G(d,p) level of theory using Gaussian-16 program.

ST8a : Optimised coordinates of systems with bdpsq fusion scheme

bdpsq-1-enNMe2			
C	-6.566588	-0.389171	0.014152
C	-6.164684	-1.720152	0.017146
C	-4.758321	-1.738697	0.014526
C	-4.320458	-0.409313	0.009848
N	-5.454754	0.390933	0.009793
H	-5.418021	1.401567	0.006693
H	-7.554790	0.042020	0.014810
H	-6.824129	-2.573472	0.020853
H	-4.112751	-2.602790	0.015830
C	-3.045640	0.187381	0.005747
C	-2.638918	1.619264	-0.000844
C	-1.682370	-0.183904	0.002709
C	-1.204559	1.169437	-0.004805
O	-3.243750	2.669992	-0.003123
O	-0.987283	-1.261274	0.002333
C	0.129041	1.459117	-0.017262
C	0.921722	2.642894	-0.034836
N	0.996567	0.348824	-0.019415
C	2.231873	2.248401	-0.048078

bdpsq-1-enPY5			
C	-7.014888	-0.670232	-0.000081
C	-6.535460	-1.976945	0.000047
C	-5.132414	-1.913142	0.000118
C	-4.772827	-0.558826	0.000014
N	-5.953033	0.173681	-0.000089
H	-5.976514	1.184917	-0.000187
H	-8.027198	-0.298939	-0.000169
H	-7.144268	-2.867016	0.000085
H	-4.436833	-2.737541	0.000222
C	-3.537338	0.108917	0.000024
C	-3.212051	1.562817	-0.000066
C	-2.152534	-0.184347	0.000056
C	-1.756794	1.192636	0.000073
O	-3.876277	2.576274	-0.000215
O	-1.398949	-1.219155	0.000152
C	-0.439688	1.563432	0.000160
C	0.277627	2.792707	0.000101
N	0.489390	0.507765	0.000156
C	1.610694	2.476139	0.000033

H	0.530805	3.648683	-0.040455
C	2.268841	0.804944	-0.036859
H	3.095154	2.895127	-0.069614
B	0.539726	-1.166934	0.011417
F	0.990911	-1.766323	1.176394
F	1.007407	-1.819093	-1.118489
C	3.398643	-0.064220	-0.039936
C	4.686127	0.392658	-0.025542
H	3.193742	-1.125000	-0.049460
H	4.880747	1.458771	0.025961
N	5.807304	-0.363602	-0.086873
C	5.719644	-1.817092	-0.123383
H	6.696142	-2.225167	-0.384299
H	5.411000	-2.230364	0.844970
H	4.998869	-2.132355	-0.880090
C	7.105906	0.218404	0.219582
H	7.421836	-0.013149	1.244982
H	7.862109	-0.165190	-0.470076
H	7.058674	1.302210	0.110451

H	-0.173671	3.772822	0.000104
C	1.730390	1.042051	0.000070
H	2.437194	3.168969	-0.000008
B	0.123919	-1.038008	0.000015
F	0.614493	-1.630689	1.148532
F	0.614234	-1.630387	-1.148766
C	2.920402	0.241173	0.000043
C	4.176572	0.750609	0.000014
H	2.775303	-0.831653	0.000036
H	4.306779	1.829878	-0.000001
C	5.393809	-0.017698	0.000005
C	6.672201	0.532055	0.000035
C	5.563993	-1.444871	-0.000129
N	7.573867	-0.491201	-0.000050
H	6.986591	1.563579	0.000115
C	6.908080	-1.701640	-0.000094
H	4.782817	-2.188132	-0.000206
H	8.574507	-0.380988	0.000077
H	7.448755	-2.633841	-0.000190

bdpsq-1-enPY6

C	-7.241618	-0.765295	-0.001024
C	-6.732566	-2.063311	-0.000587
C	-5.334341	-1.968202	0.000019
C	-5.004570	-0.603721	-0.000037
N	-6.202487	0.102149	-0.000671
H	-6.250872	1.112773	-0.000876
H	-8.262764	-0.418652	-0.001578
H	-7.322058	-2.966163	-0.000734
H	-4.619928	-2.776398	0.000420
C	-3.787141	0.087140	0.000563
C	-3.487860	1.549469	0.000400
C	-2.393987	-0.179051	0.000983
C	-2.028791	1.202745	0.000918
O	-4.171015	2.548603	-0.000073
O	-1.623001	-1.199934	0.001003
C	-0.715395	1.602988	0.000352
C	-0.024273	2.844224	0.000005
N	0.229335	0.565598	0.000404
C	1.317293	2.551529	-0.000121
H	-0.493151	3.815919	-0.000077
C	1.459183	1.124748	0.000128
H	2.131099	3.259115	-0.000302
B	-0.104681	-0.990776	0.000227
F	0.400035	-1.568707	1.148251
F	0.398792	-1.568050	-1.148700
C	2.663754	0.333822	0.000099
C	3.909514	0.853666	-0.000146
H	2.520745	-0.739175	0.000364
H	4.030372	1.933428	-0.000352
C	5.159006	0.097520	-0.000089
C	5.228645	-1.305762	0.000347
C	6.381265	0.786816	-0.000646
C	6.472788	-1.922643	0.000167

bdpsq-1-NMe2

C	-5.849090	-0.063682	0.155224
C	-5.540392	-1.416088	0.240641
C	-4.139845	-1.536193	0.181346
C	-3.612235	-0.246147	0.060105
N	-4.686989	0.631841	0.046987
H	-4.582066	1.634500	-0.030907
H	-6.803907	0.436978	0.164218
H	-6.256082	-2.217321	0.334565
H	-3.556636	-2.442763	0.219461
C	-2.299196	0.253849	-0.042597
C	-1.790585	1.648429	-0.149452
C	-0.967835	-0.213440	-0.047986
C	-0.390425	1.092734	-0.152036
O	-2.313477	2.740554	-0.194340
O	-0.339463	-1.327912	0.052094
C	0.954823	1.293030	-0.132346
C	1.781241	2.444654	-0.052855
N	1.776586	0.132380	-0.067644
C	3.069289	2.012271	0.078547
H	1.424265	3.462448	-0.086253
C	3.057579	0.563798	0.055394
H	3.952704	2.624863	0.145134
B	1.174007	-1.343329	-0.104934
F	1.692311	-2.079905	0.943637
F	1.432989	-1.923859	-1.344582
N	4.174058	-0.190078	0.136939
C	4.284996	-1.594373	-0.266862
H	5.246094	-1.723046	-0.770992
H	4.238639	-2.259994	0.598229
H	3.495700	-1.862904	-0.960256
C	5.430557	0.433704	0.547732
H	6.049261	-0.324816	1.028896
H	5.984215	0.840572	-0.307319

H	4.334018	-1.915911	0.000834
C	7.574938	0.071690	-0.000702
H	6.400606	1.871286	-0.000995
N	7.638477	-1.262270	-0.000352
H	6.539919	-3.006654	0.000412
H	8.525768	0.597205	-0.001096

H	5.254727	1.226577	1.273264

bdpsq-1-PY5

C	-6.259238	-0.350218	-0.081838
C	-5.864181	-1.684308	-0.117110
C	-4.460144	-1.710865	-0.089407
C	-4.015214	-0.383375	-0.037429
N	-5.146013	0.423185	-0.034205
H	-5.105398	1.433320	-0.001168
H	-7.245634	0.085226	-0.087670
H	-6.528303	-2.532914	-0.157978
H	-3.818735	-2.577964	-0.104200
C	-2.739522	0.202879	0.007936
C	-2.321221	1.631801	0.056289
C	-1.376792	-0.178387	0.016379
C	-0.892435	1.166781	0.063418
O	-2.917389	2.686392	0.074946
O	-0.685037	-1.253800	-0.018081
C	0.442498	1.457693	0.068227
C	1.207667	2.653470	0.057640
N	1.325822	0.353489	0.044687
C	2.523301	2.277731	0.022164
H	0.797342	3.651142	0.077138
C	2.585560	0.840309	0.015888
H	3.381508	2.930673	0.022275
B	0.844523	-1.166862	0.045069
F	1.226634	-1.773719	1.230171
F	1.333705	-1.811688	-1.070661
C	3.817078	0.086192	-0.012397
C	5.052316	0.673049	-0.292330
C	4.073279	-1.306768	0.227118
N	6.002333	-0.296179	-0.231167
H	5.306814	1.688237	-0.547278
C	5.418604	-1.507478	0.088298
H	3.347438	-2.056022	0.485828
H	6.983299	-0.152594	-0.406898
H	6.011072	-2.401371	0.191818

bdpsq-1-PY6

C	-6.435761	-0.465754	-0.255106
C	-5.997826	-1.785128	-0.370500
C	-4.599676	-1.773826	-0.288371
C	-4.197737	-0.438569	-0.122112
N	-5.354513	0.333419	-0.106667
H	-5.349095	1.339661	-0.000120
H	-7.435427	-0.061481	-0.269936
H	-6.634087	-2.646083	-0.498972
H	-3.930645	-2.618482	-0.339155
C	-2.947848	0.173182	0.018029
C	-2.568127	1.608806	0.173576
C	-1.571817	-0.173291	0.042236
C	-1.132276	1.176462	0.187021
O	-3.193793	2.642396	0.239677
O	-0.852848	-1.224674	-0.060800
C	0.199889	1.510920	0.201064
C	0.928239	2.724394	0.182722
N	1.104818	0.431756	0.121509
C	2.256052	2.381644	0.071427
H	0.494539	3.710738	0.237250
C	2.345752	0.956612	0.042271
H	3.102753	3.049096	0.043546
B	0.663092	-1.104562	0.153302
F	0.922070	-1.623464	1.413222
F	1.279166	-1.791612	-0.860574
C	3.610425	0.212566	-0.047887
C	3.866741	-0.973832	0.649521
C	4.649330	0.733057	-0.834087
C	5.120875	-1.565302	0.526093
H	3.116832	-1.425078	1.283108
C	5.862019	0.055620	-0.892151
H	4.509615	1.637808	-1.413155
N	6.111546	-1.075413	-0.225458
H	5.338079	-2.483383	1.063924
H	6.671496	0.440214	-1.506019

bdpsq-2-enNMe2-geo

C	6.319127	-1.709500	-0.024694
C	6.607805	-0.347780	0.014906
C	5.386218	0.343445	0.027584
C	4.361260	-0.612548	-0.004665
N	4.971986	-1.860234	-0.036185
H	4.454614	-2.729074	-0.063314
H	6.979777	-2.561461	-0.044907

bdpsq-2-enPY5

C	6.781031	-1.899774	0.000145
C	7.123682	-0.548899	0.000224
C	5.931419	0.189303	0.000123
C	4.868771	-0.726838	0.000035
N	5.430369	-1.998443	0.000090
H	4.879506	-2.847088	0.000081
H	7.408324	-2.776893	0.000169

H	7.596655	0.081977	0.032324
H	5.234836	1.411024	0.056729
C	2.961386	-0.520731	-0.009500
C	1.910811	-1.576742	-0.046579
C	1.945670	0.466586	0.010134
C	0.878012	-0.488696	-0.026227
O	1.933506	-2.787872	-0.079923
O	1.870290	1.743918	0.042050
C	-0.441254	-0.110672	-0.037181
C	-1.705930	-0.737176	-0.094953
N	-0.636244	1.289240	-0.005694
C	-2.672758	0.269191	-0.092047
H	-1.854789	-1.804022	-0.150980
C	-1.944515	1.502300	-0.039904
B	0.489015	2.408789	0.078218
F	0.371922	3.081497	1.277054
F	0.384468	3.239796	-1.016754
C	-4.118257	0.209279	-0.124199
C	-4.831962	-0.939813	-0.012226
H	-4.632420	1.156243	-0.240374
H	-4.309070	-1.874976	0.166029
N	-6.187703	-1.090538	-0.126703
C	-7.027920	0.078562	-0.311824
H	-8.038911	-0.243355	-0.564623
H	-7.076295	0.705805	0.590724
H	-6.645750	0.686572	-1.134660
C	-6.817116	-2.255888	0.477566
H	-7.087360	-2.085538	1.529800
H	-7.723732	-2.515492	-0.073945
H	-6.134507	-3.105869	0.432840
H	-2.345744	2.506033	-0.023536

H	8.128835	-0.158534	0.000302
H	5.821913	1.262403	0.000119
C	3.475673	-0.579823	-0.000091
C	2.383290	-1.594510	-0.000135
C	2.498788	0.448390	-0.000108
C	1.396581	-0.465552	-0.000175
O	2.358880	-2.805496	-0.000107
O	2.474370	1.726963	-0.000058
C	0.091894	-0.034497	-0.000079
C	-1.194093	-0.615160	-0.000112
N	-0.049995	1.371811	-0.000037
C	-2.121593	0.427700	0.000004
H	-1.386697	-1.676360	-0.000146
C	-1.350812	1.633188	-0.000012
B	1.118389	2.449654	-0.000068
F	1.040465	3.205215	1.149724
F	1.040485	3.205261	-1.149783
C	-3.570294	0.409839	0.000064
C	-4.343655	-0.696308	-0.000089
H	-4.048725	1.385375	0.000224
H	-3.857714	-1.669634	-0.000309
C	-5.789683	-0.729971	-0.000015
C	-6.548215	-1.893395	-0.000071
C	-6.723373	0.361402	0.000191
N	-7.870372	-1.542762	0.000025
H	-6.238274	-2.926224	-0.000219
C	-7.986954	-0.169309	0.000218
H	-6.489369	1.414121	0.000385
H	-8.641088	-2.189902	-0.000041
H	-8.953051	0.308414	0.000344
H	-1.714920	2.651044	0.000041

bdpsq-2-enPY6

C	7.017281	-1.967479	-0.000564
C	7.379377	-0.619557	-0.000880
C	6.199483	0.133537	-0.000765
C	5.122668	-0.769250	-0.000378
N	5.667844	-2.049295	-0.000231
H	5.106724	-2.891499	0.000040
H	7.633980	-2.852226	-0.000547
H	8.390061	-0.243961	-0.001172
H	6.104107	1.208034	-0.000939
C	3.735753	-0.601620	-0.000136
C	2.624873	-1.599277	0.000338
C	2.773101	0.443851	-0.000155
C	1.660765	-0.453475	0.000224
O	2.581139	-2.808701	0.000669
O	2.769793	1.721426	-0.000421
C	0.360203	0.000582	0.000377
C	-0.930503	-0.563307	0.000255
N	0.238678	1.406728	0.000192
C	-1.842277	0.495352	0.000034
H	-1.138817	-1.621578	0.000283

bdpsq-2-NMe2

C	5.812344	-0.961152	0.037094
C	5.867552	0.430293	0.036881
C	4.547059	0.905968	0.024665
C	3.697895	-0.209454	0.017497
N	4.509990	-1.336869	0.025593
H	4.146766	-2.280984	0.022500
H	6.607010	-1.689957	0.044613
H	6.769806	1.020774	0.044726
H	4.218247	1.933279	0.021158
C	2.302461	-0.354933	0.004910
C	1.445215	-1.573874	-0.004996
C	1.135386	0.446434	-0.009492
C	0.243317	-0.675099	-0.021104
O	1.671256	-2.764066	-0.002251
O	0.845294	1.693907	-0.016827
C	-1.119949	-0.526054	-0.047688
C	-2.260690	-1.362767	-0.063824
N	-1.545637	0.817307	-0.058085
C	-3.376105	-0.526120	-0.099110
H	-2.232997	-2.439284	-0.050775

C	-1.059005	1.689015	-0.000024
B	1.424003	2.468446	0.000524
F	1.359072	3.220918	1.151107
F	1.358272	3.222527	-1.148921
C	-3.291831	0.489820	-0.000183
C	-4.075046	-0.606191	0.000149
H	-3.754323	1.472791	-0.000627
H	-3.601565	-1.584734	0.000724
C	-5.537180	-0.634089	-0.000108
C	-6.351094	0.511274	-0.001363
C	-6.203344	-1.869038	0.000953
C	-7.732095	0.367315	-0.001454
H	-5.924900	1.507054	-0.002316
C	-7.594489	-1.904541	0.000756
H	-5.639859	-2.795822	0.001943
N	-8.364784	-0.813449	-0.000411
H	-8.368533	1.247770	-0.002416
H	-8.114708	-2.858406	0.001590
H	-1.407749	2.712117	-0.000142
C	-2.872743	0.818513	-0.086727
B	-0.624872	2.115585	-0.015912
F	-0.874987	2.805021	1.152742
F	-0.859360	2.870763	-1.145095
N	-4.708427	-0.875454	-0.176768
C	-5.033881	-2.279476	0.014490
H	-4.841862	-2.622181	1.043047
H	-6.088521	-2.436412	-0.213668
H	-4.446660	-2.895863	-0.669394
C	-5.711279	0.086498	0.262342
H	-6.697461	-0.269812	-0.037430
H	-5.709364	0.235107	1.352437
H	-5.553222	1.051947	-0.220238
H	-3.421632	1.747124	-0.098421

bdpsq-2-PY5

C	6.233552	-1.232571	-0.046471
C	6.370763	0.154140	-0.041253
C	5.081565	0.706097	-0.025038
C	4.167839	-0.358219	-0.020602
N	4.912707	-1.531709	-0.034039
H	4.494851	-2.453120	-0.034118
H	6.984640	-2.006238	-0.058062
H	7.306337	0.690206	-0.048433
H	4.813194	1.750828	-0.017055
C	2.767973	-0.420632	-0.006174
C	1.839693	-1.586785	-0.003585
C	1.649533	0.450473	0.008022
C	0.695114	-0.617675	0.009545
O	1.995432	-2.787980	-0.010718
O	1.433556	1.710955	0.014159
C	-0.657590	-0.384913	0.013304
C	-1.846282	-1.149931	-0.004793
N	-1.009068	0.982076	0.018504
C	-2.914787	-0.259045	-0.007882
H	-1.883323	-2.227804	-0.028164
C	-2.335380	1.048034	0.006717
B	-0.015120	2.221824	0.056055
F	-0.187092	2.908268	1.239012
F	-0.222437	3.004919	-1.058198
C	-4.342199	-0.536244	-0.018139
C	-4.947418	-1.763604	0.201675
C	-5.398764	0.402779	-0.258048
N	-6.301919	-1.591826	0.100056
H	-4.521846	-2.726156	0.433542
C	-6.588977	-0.276329	-0.179715
H	-5.292836	1.453437	-0.478182
H	-6.985542	-2.320159	0.223599

bdpsq-2-PY6

C	6.437894	-1.324998	-0.116189
C	6.604072	0.060713	-0.096719
C	5.329283	0.637165	-0.056248
C	4.392551	-0.410216	-0.051526
N	5.114477	-1.599009	-0.089210
H	4.679624	-2.512831	-0.094286
H	7.174297	-2.112316	-0.147100
H	7.550593	0.576898	-0.110481
H	5.081723	1.686827	-0.032097
C	2.996329	-0.442202	-0.017846
C	2.039148	-1.588094	-0.017873
C	1.895325	0.455236	0.020459
C	0.921947	-0.591372	0.019046
O	2.167548	-2.791079	-0.041708
O	1.708839	1.719092	0.041294
C	-0.428871	-0.325415	0.032163
C	-1.629772	-1.065653	0.004023
N	-0.751043	1.046011	0.052972
C	-2.678334	-0.148741	0.001057
H	-1.691147	-2.141723	-0.038272
C	-2.076547	1.143751	0.032116
B	0.271566	2.262898	0.134718
F	0.137621	2.887962	1.354207
F	0.063631	3.101712	-0.935046
C	-4.118899	-0.423214	-0.025923
C	-5.042847	0.526206	-0.483813
C	-4.639374	-1.652507	0.401547
C	-6.398211	0.211560	-0.491417
H	-4.718317	1.493004	-0.849943
C	-6.012018	-1.868268	0.348543
H	-3.989210	-2.427827	0.788973
N	-6.893572	-0.961813	-0.086730

H	-7.604567	0.062002	-0.302527
H	-2.841318	2.002169	0.017235

H	-7.122019	0.939822	-0.846211
H	-6.425712	-2.816956	0.678787
H	-2.559111	2.109400	0.060275

bdpsq-3-enNMe2

C	4.518491	-3.062310	-0.052208
C	5.323947	-1.929742	-0.071460
C	4.477377	-0.806695	-0.058894
C	3.159021	-1.274653	-0.031894
N	3.220430	-2.661228	-0.028615
H	2.401129	-3.252570	-0.010508
H	4.782992	-4.107540	-0.053703
H	6.402130	-1.928127	-0.092047
H	4.764628	0.232955	-0.067413
C	1.911636	-0.621669	-0.008736
C	0.533937	-1.147811	0.016233
C	1.396569	0.695584	-0.007515
C	0.017635	0.267859	0.008740
O	0.057845	-2.270588	0.034610
O	1.860667	1.883479	-0.026896
C	-1.013216	1.163202	-0.015278
C	-2.466483	1.136887	-0.059787
N	-0.596856	2.517220	-0.037693
C	-2.851529	2.486875	-0.112910
C	-1.697318	3.274641	-0.095745
B	0.875264	3.063928	0.069975
F	1.069356	3.660301	1.302275
F	1.135962	3.918896	-0.980212
C	-3.376307	0.036279	-0.059556
C	-3.023792	-1.284869	0.004188
H	-4.424229	0.308653	-0.111314
H	-1.982497	-1.575706	0.081016
N	-3.865992	-2.342112	-0.036096
C	-5.305618	-2.158932	-0.112429
H	-5.777922	-3.119663	-0.316621
H	-5.715364	-1.760172	0.824561
H	-5.560676	-1.470925	-0.922562
C	-3.367050	-3.685588	0.233073
H	-3.683598	-4.035843	1.223452
H	-3.743859	-4.385986	-0.517956
H	-2.278444	-3.681028	0.195875
H	-1.619420	4.352049	-0.121034
H	-3.864016	2.856857	-0.159992

bdpsq-3-enPY5

C	4.505737	-3.847945	0.000187
C	5.514415	-2.887636	0.000169
C	4.897968	-1.626913	0.000041
C	3.511698	-1.836202	-0.000018
N	3.309368	-3.210905	0.000043
H	2.391535	-3.635907	0.000046
H	4.568765	-4.924405	0.000292
H	6.573152	-3.092181	0.000252
H	5.376986	-0.660440	0.000006
C	2.410595	-0.966985	-0.000194
C	0.947557	-1.239754	-0.000199
C	2.136654	0.424833	-0.000258
C	0.714288	0.240780	-0.000255
O	0.273204	-2.248346	-0.000169
O	2.791670	1.521320	-0.000222
C	-0.147467	1.303675	-0.000101
C	-1.573018	1.472909	-0.000082
N	0.466760	2.567023	-0.000149
C	-1.776337	2.860820	0.000027
C	-0.516479	3.477776	-0.000049
B	2.019915	2.860578	0.000064
F	2.366590	3.538887	1.149632
F	2.366853	3.539608	-1.148939
C	-2.501222	0.373975	-0.000116
C	-3.850128	0.493567	-0.000115
H	-2.059709	-0.618577	-0.000090
H	-4.285409	1.490342	-0.000061
C	-4.793516	-0.596568	-0.000025
C	-6.175872	-0.443404	0.000229
C	-4.541139	-2.011614	-0.000075
N	-6.741764	-1.685922	0.000228
H	-6.777109	0.451782	0.000347
C	-5.752746	-2.649233	-0.000043
H	-3.577284	-2.495564	-0.000250
H	-7.731087	-1.871433	0.000419
H	-5.998288	-3.698605	-0.000042
H	-0.288276	4.533747	-0.000052
H	-2.719308	3.384261	0.000119

bdpsq-3-enPY6

C	4.470921	-4.044654	0.000029
C	5.537722	-3.145869	0.000315
C	4.999537	-1.852920	0.000351
C	3.600676	-1.978255	0.000122
N	3.316275	-3.339690	-0.000067
H	2.375288	-3.711234	-0.000274
H	4.470709	-5.123082	-0.000091

bdpsq-3-NMe2

C	5.285267	-1.211453	-0.076284
C	5.474583	0.163688	-0.156461
C	4.205216	0.768027	-0.138799
C	3.254623	-0.254776	-0.047648
N	3.950983	-1.454979	-0.011741
H	3.498178	-2.356436	0.055524
H	6.003731	-2.015260	-0.061016

H	6.581824	-3.414963	0.000462
H	5.535479	-0.916751	0.000530
C	2.559485	-1.044558	0.000050
C	1.079032	-1.220463	-0.000194
C	2.374261	0.365327	0.000128
C	0.946889	0.269260	-0.000020
O	0.339082	-2.180991	-0.000491
O	3.097151	1.416848	0.000291
C	0.149281	1.386218	-0.000071
C	-1.258454	1.641120	-0.000009
N	0.837771	2.606090	0.000022
C	-1.381253	3.036421	0.000129
C	-0.085341	3.577986	0.000151
B	2.411155	2.804120	-0.000123
F	2.794504	3.456795	1.149492
F	2.794503	3.455976	-1.150192
C	-2.252703	0.594258	-0.000053
C	-3.588044	0.787025	0.000118
H	-1.859479	-0.418349	-0.000220
H	-3.970098	1.804677	0.000345
C	-4.611050	-0.256283	0.000090
C	-4.330563	-1.633539	-0.000108
C	-5.966812	0.105733	0.000227
C	-5.382099	-2.540405	-0.000153
H	-3.312534	-2.003516	-0.000225
C	-6.945109	-0.883889	0.000174
H	-6.255782	1.151177	0.000377
N	-6.675833	-2.192062	-0.000019
H	-5.176940	-3.607117	-0.000321
H	-7.996679	-0.610795	0.000290
H	0.207565	4.617610	0.000224
H	-2.291792	3.614506	0.000218

H	6.428802	0.662029	-0.219612
H	3.977966	1.821462	-0.184661
C	1.847919	-0.253279	0.009641
C	0.881275	-1.362575	0.097481
C	0.782567	0.672003	-0.004543
C	-0.245216	-0.342815	0.067780
O	0.996998	-2.569750	0.160776
O	0.653090	1.940823	-0.079323
C	-1.570405	-0.002377	0.025813
C	-2.865982	-0.664674	-0.038880
N	-1.810788	1.390687	-0.077213
C	-3.818787	0.358231	-0.209878
C	-3.126842	1.570129	-0.216858
B	-0.750158	2.538499	0.093755
F	-0.819416	3.061286	1.374183
F	-0.938504	3.493755	-0.881325
N	-3.116865	-1.989508	0.041373
C	-2.037417	-2.958443	0.166225
H	-1.356135	-2.679529	0.970427
H	-2.459886	-3.933831	0.401995
H	-1.450019	-3.044011	-0.753559
C	-4.482865	-2.451036	-0.168397
H	-4.527977	-3.524332	0.005209
H	-5.167881	-1.960190	0.529455
H	-4.824312	-2.246789	-1.190388
H	-3.533820	2.566205	-0.314645
H	-4.884187	0.246918	-0.316919

bdpsq-3-PY5

C	5.100527	-2.248159	-0.028963
C	5.639297	-0.964976	-0.062070
C	4.569018	-0.056498	-0.054888
C	3.383849	-0.803171	-0.017600
N	3.748774	-2.143285	-0.002627
H	3.079026	-2.900338	0.024013
H	5.589422	-3.209222	-0.022766
H	6.690990	-0.728283	-0.087861
H	4.620307	1.020785	-0.073685
C	2.027133	-0.442179	0.005648
C	0.798462	-1.264570	0.039163
C	1.230771	0.727647	-0.002361
C	-0.014475	0.003598	0.024029
O	0.592193	-2.463037	0.064734
O	1.422604	1.988403	-0.034414
C	-1.222463	0.649471	0.000645
C	-2.624299	0.302389	-0.029344
N	-1.114705	2.060116	-0.034217
C	-3.303441	1.521500	-0.084164

bdpsq-3-PY6

C	4.963440	-2.683579	-0.171350
C	5.644953	-1.467722	-0.238252
C	4.689111	-0.445839	-0.190288
C	3.426536	-1.053834	-0.093550
N	3.638382	-2.428565	-0.084998
H	2.888444	-3.105239	-0.023079
H	5.341951	-3.693386	-0.180358
H	6.714555	-1.354045	-0.312886
H	4.861076	0.618691	-0.219236
C	2.126664	-0.546105	-0.011286
C	0.812326	-1.236336	0.079388
C	1.457153	0.704024	0.002746
C	0.150553	0.115397	0.071546
O	0.483274	-2.400161	0.134741
O	1.780583	1.938050	-0.050082
C	-0.989295	0.890373	0.051799
C	-2.406134	0.690258	-0.028717
N	-0.734345	2.274156	-0.016492
C	-2.959792	1.963430	-0.152570

C	-2.351868	2.554125	-0.084163
B	0.204976	2.925051	0.039622
F	0.262063	3.585529	1.250707
F	0.260549	3.779731	-1.039586
C	-3.232651	-1.007761	-0.012963
C	-2.598376	-2.244748	0.042247
C	-4.645186	-1.273619	-0.049942
N	-3.563036	-3.207297	0.039048
H	-1.551329	-2.506023	0.078869
C	-4.815507	-2.631238	-0.016459
H	-5.438332	-0.544617	-0.094676
H	-3.379540	-4.196795	0.072389
H	-5.709266	-3.232927	-0.026939
H	-2.518516	3.621063	-0.116508
H	-4.371515	1.663222	-0.121920

C	-1.907296	2.897822	-0.134647
B	0.673075	2.990018	0.123442
F	0.795994	3.516947	1.392544
F	0.808915	3.928260	-0.871460
C	-3.141002	-0.578550	-0.006664
C	-4.367292	-0.703865	-0.677662
C	-2.682620	-1.703832	0.688512
C	-5.056540	-1.909180	-0.618711
H	-4.769704	0.118430	-1.256863
C	-3.448868	-2.866042	0.679495
H	-1.749912	-1.689052	1.234900
N	-4.619046	-2.984463	0.045787
H	-6.005444	-2.019171	-1.136050
H	-3.100948	-3.745604	1.212967
H	-1.958572	3.974938	-0.193316
H	-4.008163	2.207956	-0.219122

bdpsq-4-enNMe2

C	-3.112868	-0.322417	-0.059142
C	-2.739116	-1.693843	-0.078285
C	-1.355524	-1.769988	-0.064502
C	-0.848763	-0.451821	-0.039638
N	-1.957488	0.394033	-0.038597
H	-1.873824	1.402349	-0.017572
H	-3.423131	-2.527062	-0.107561
H	-0.746958	-2.660957	-0.075317
C	0.433328	0.071804	-0.019640
C	0.922137	1.486424	0.005722
C	1.793637	-0.362057	-0.011713
C	2.317220	0.960323	0.012209
O	0.362320	2.562817	0.015787
O	2.425501	-1.474083	-0.021333
C	3.680593	1.200408	0.027701
C	4.530707	2.326269	0.049258
N	4.474926	0.041539	0.018954
C	5.833843	1.841651	0.053277
C	5.756367	0.434296	0.034318
B	3.967784	-1.455164	-0.001369
F	4.375856	-2.103401	1.147464
F	4.405842	-2.082296	-1.150666
C	-4.395168	0.316014	-0.055793
C	-5.570353	-0.374436	-0.014933
H	-4.399281	1.399288	-0.082950
H	-5.546045	-1.456814	0.058208
N	-6.824735	0.140593	-0.077855
C	-7.027001	1.579173	-0.132779
H	-8.070452	1.784470	-0.371758
H	-6.784013	2.065605	0.821631
H	-6.403694	2.017297	-0.915546
C	-7.966666	-0.677529	0.308144
H	-8.256702	-0.507720	1.353390
H	-8.822829	-0.448667	-0.330770
H	-7.720137	-1.732682	0.186497
H	6.557540	-0.289320	0.031382

bdpsq-4-enPY5

C	-2.533300	-1.377312	-0.000357
C	-1.908056	-2.647063	-0.000799
C	-0.531676	-2.459958	-0.000658
C	-0.294010	-1.069873	-0.000336
N	-1.538540	-0.448304	-0.000137
H	-1.640406	0.557723	0.000119
H	-2.436341	-3.587902	-0.001110
H	0.237923	-3.215971	-0.000816
C	0.866957	-0.304730	-0.000176
C	1.066944	1.176443	0.000309
C	2.282453	-0.469123	-0.000256
C	2.541069	0.933536	0.000020
O	0.310268	2.123741	0.000784
O	3.118438	-1.435482	-0.000543
C	3.827769	1.433148	0.000007
C	4.443748	2.705593	-0.000602
N	4.834448	0.450850	-0.000468
C	5.813404	2.484394	-0.001166
C	6.011687	1.085660	-0.001192
B	4.628386	-1.119368	0.000691
F	5.165420	-1.657102	1.151293
F	5.167957	-1.659158	-1.147665
C	-3.940358	-1.092655	-0.000312
C	-4.502731	0.139503	0.000097
H	-4.577520	-1.970581	-0.000687
H	-3.856018	1.014722	0.000407
C	-5.914350	0.431599	0.000060
C	-6.448866	1.715505	0.000552
C	-7.030786	-0.472889	-0.000442
N	-7.809536	1.609647	0.000614
H	-5.955689	2.674463	0.000958
C	-8.175169	0.279323	-0.000170
H	-6.992651	-1.550534	-0.001030
H	-8.450097	2.386371	0.000855
H	-9.212296	-0.013432	-0.000395
H	6.939498	0.533371	-0.001661

H	6.745532	2.418302	0.067912
H	4.204062	3.354363	0.059758

H	6.596091	3.226811	-0.001616
H	3.922558	3.650105	-0.000590

bdpsq-4-enPY6

C	-2.237886	-1.442243	-0.000288
C	-1.600766	-2.701285	-0.000452
C	-0.224094	-2.496421	-0.000411
C	-0.007757	-1.105429	-0.000071
N	-1.254900	-0.498286	-0.000014
H	-1.369583	0.506765	0.000255
H	-2.116536	-3.649069	-0.000632
H	0.554931	-3.242509	-0.000558
C	1.147954	-0.321455	0.000158
C	1.322774	1.160077	0.000400
C	2.561133	-0.471730	0.000071
C	2.804455	0.938511	0.000265
O	0.554861	2.096437	0.000549
O	3.408695	-1.426129	-0.000317
C	4.079646	1.452706	-0.000131
C	4.680807	2.736293	-0.000404
N	5.101525	0.483005	-0.000428
C	6.049343	2.533137	-0.000937
C	6.266220	1.132939	-0.000917
B	4.916076	-1.093686	0.000428
F	5.458641	-1.619743	1.151079
F	5.460166	-1.621144	-1.148828
C	-3.650382	-1.173385	-0.000286
C	-4.229882	0.046602	-0.000126
H	-4.268714	-2.064552	-0.000351
H	-3.599152	0.932503	0.000055
C	-5.662879	0.328733	-0.000063
C	-6.662041	-0.659281	-0.000372
C	-6.102313	1.661458	0.000332
C	-7.996915	-0.277204	-0.000239
H	-6.415298	-1.713916	-0.000753
C	-7.466272	1.937588	0.000424
H	-5.386372	2.476149	0.000572
N	-8.413229	0.995838	0.000159
H	-8.777176	-1.032951	-0.000472
H	-7.813520	2.966878	0.000737
H	7.202571	0.594794	-0.001216
H	6.823223	3.284638	-0.001309
H	4.146884	3.673664	-0.000322

bdpsq-4-NMe2

C	-3.951934	-0.330209	0.067020
C	-3.614024	-1.710720	0.052879
C	-2.228595	-1.805003	0.044477
C	-1.696364	-0.502003	0.044664
N	-2.793730	0.375961	0.052579
H	-2.674872	1.380410	0.044415
H	-4.314205	-2.528724	0.048282
H	-1.639126	-2.708651	0.035319
C	-0.414104	0.014087	0.030803
C	0.060731	1.432053	0.027371
C	0.951776	-0.405408	0.014186
C	1.459777	0.923290	0.011301
O	-0.518047	2.500352	0.034470
O	1.595191	-1.509930	0.005341
C	2.820823	1.179532	-0.000563
C	3.657848	2.314802	-0.000775
N	3.627881	0.029689	-0.011321
C	4.966655	1.844989	-0.011499
C	4.905149	0.437137	-0.017807
B	3.138942	-1.472641	-0.022767
F	3.589311	-2.121379	1.108913
F	3.545367	-2.089478	-1.188993
N	-5.177046	0.257719	0.115810
C	-5.290584	1.695892	-0.096046
H	-5.072219	1.985498	-1.132632
H	-6.306268	2.007275	0.144264
H	-4.616797	2.237632	0.572069
C	-6.358291	-0.563732	-0.123347
H	-7.239049	-0.020777	0.219107
H	-6.486194	-0.811492	-1.185056
H	-6.294145	-1.489515	0.448755
H	5.714362	-0.277401	-0.026780
H	5.871683	2.432184	-0.014267
H	3.319963	3.339290	0.007128

bdpsq-4-PY5

C	-3.429803	-0.605741	-0.000191
C	-3.003027	-1.953204	-0.000584
C	-1.613236	-1.970116	-0.000610
C	-1.170373	-0.632216	-0.000295
N	-2.312571	0.164538	-0.000023
H	-2.271792	1.175371	0.000512
H	-3.656289	-2.811243	-0.000979

bdpsq-4-PY6

C	-3.168442	-0.684188	0.023017
C	-2.728318	-2.020058	0.066827
C	-1.334288	-2.019874	0.076353
C	-0.913894	-0.679181	0.034414
N	-2.058381	0.103292	0.009298
H	-2.027186	1.112029	-0.065881
H	-3.368701	-2.886148	0.111158

H	-0.965751	-2.833056	-0.000917
C	0.089095	-0.044609	-0.000180
C	0.503163	1.391616	0.000202
C	1.465344	-0.413530	-0.000232
C	1.925671	0.935825	0.000089
O	-0.107918	2.438657	0.000490
O	2.151151	-1.492194	-0.000484
C	3.271762	1.242332	0.000196
C	4.066793	2.410919	0.000297
N	4.124000	0.123464	-0.000070
C	5.389607	1.991937	0.000118
C	5.381450	0.579489	-0.000141
B	3.690806	-1.399603	0.000028
F	4.144472	-2.011403	1.149792
F	4.145313	-2.011831	-1.149138
C	-4.761897	-0.051663	-0.000046
C	-5.943884	-0.780758	0.001552
C	-5.133003	1.334444	-0.001464
N	-6.981868	0.105350	0.001071
H	-6.113276	-1.844676	0.003181
C	-6.502407	1.396007	-0.000777
H	-4.473484	2.188365	-0.003109
H	-7.955946	-0.149973	0.002002
H	-7.170003	2.241571	-0.001471
H	6.218593	-0.102439	-0.000344
H	6.272268	2.612177	0.000146
H	3.689259	3.421479	0.000471

H	-0.676594	-2.873934	0.116138
C	0.344747	-0.070917	0.009850
C	0.730863	1.368281	-0.043114
C	1.719970	-0.424848	0.016781
C	2.165607	0.934871	-0.033552
O	0.106286	2.404872	-0.078559
O	2.420395	-1.491477	0.051289
C	3.500867	1.258367	-0.052185
C	4.281996	2.440677	-0.100551
N	4.371820	0.151141	-0.016566
C	5.606009	2.041394	-0.093883
C	5.617601	0.624880	-0.041608
B	3.959620	-1.381676	0.044686
F	4.422816	-1.934658	1.216952
F	4.419799	-2.025660	-1.081244
C	-4.524492	-0.146909	0.010660
C	-4.799584	1.197879	0.300898
C	-5.621078	-0.966635	-0.294751
C	-6.116678	1.644126	0.268210
H	-4.015058	1.894884	0.571903
C	-6.898658	-0.419346	-0.295426
H	-5.484554	-2.011353	-0.544451
N	-7.161300	0.863242	-0.022313
H	-6.342267	2.682506	0.492797
H	-7.755651	-1.042929	-0.532666
H	6.466365	-0.042703	-0.022072
H	6.480743	2.671980	-0.122609
H	3.889475	3.444898	-0.135554

bdpsq-5-enNMe2

C	-2.887405	1.676841	0.163786
C	-3.073428	0.278010	0.147193
C	-1.782030	-0.282824	0.109994
C	-0.844482	0.761472	0.091963
N	-1.567051	1.950056	0.122392
H	-1.130082	2.863094	0.131632
H	-1.534152	-1.332953	0.089698
C	0.548222	0.809638	0.052515
C	1.487890	1.970002	0.034733
C	1.667682	-0.068233	0.017181
C	2.620542	0.994601	-0.002178
O	1.336091	3.172301	0.048465
O	1.878177	-1.328824	0.005817
C	3.977098	0.751176	-0.035444
C	5.166456	1.516729	-0.056234
N	4.324749	-0.612274	-0.051063
C	6.218999	0.614833	-0.083951
C	5.658861	-0.683249	-0.079856
B	3.329526	-1.845728	-0.042809
F	3.541890	-2.603569	1.089060
F	3.477236	-2.566821	-1.208814
C	-4.325851	-0.459602	0.169992
C	-5.544270	0.092917	-0.036294

bdpsq-5-enPY5

C	-2.247375	1.928526	-0.000104
C	-2.504990	0.542098	0.000014
C	-1.245518	-0.088902	-0.000021
C	-0.254530	0.903181	-0.000044
N	-0.915086	2.128913	-0.000072
H	-0.430604	3.018006	-0.000085
H	-1.055304	-1.151236	-0.000006
C	1.140660	0.876546	-0.000073
C	2.139599	1.985420	-0.000051
C	2.210533	-0.060264	-0.000059
C	3.220188	0.950640	-0.000038
O	2.051832	3.193833	-0.000034
O	2.353313	-1.329913	-0.000019
C	4.560864	0.635519	0.000070
C	5.790392	1.336920	0.000200
N	4.835928	-0.745078	0.000071
C	6.792847	0.380734	0.000261
C	6.163692	-0.886572	0.000223
B	3.775739	-1.924883	-0.000128
F	3.916928	-2.671570	1.149425
F	3.916896	-2.671219	-1.149891
C	-3.794137	-0.128933	0.000059
C	-5.002044	0.468311	-0.000033

H	-4.239168	-1.522457	0.361984
H	-5.620361	1.145481	-0.295997
N	-6.768885	-0.521806	0.073406
C	-6.823538	-1.945122	0.353275
H	-7.854796	-2.227996	0.568879
H	-6.463482	-2.553999	-0.490093
H	-6.214488	-2.176230	1.229815
C	-7.881283	0.024829	-0.690801
H	-7.902723	-0.345603	-1.726587
H	-8.825492	-0.240638	-0.209985
H	-7.807605	1.113528	-0.718780
H	6.163352	-1.637814	-0.096454
H	7.273727	0.840405	-0.104712
H	5.213767	2.594451	-0.050210
H	-3.614870	2.471126	0.220013
H	-3.744389	-1.213962	0.000180
H	-5.050741	1.555532	-0.000148
C	-6.287420	-0.200569	0.000021
C	-7.513326	0.450087	-0.000037
C	-6.575712	-1.606994	0.000155
N	-8.501499	-0.497322	0.000031
H	-7.743134	1.503673	-0.000124
C	-7.938720	-1.754646	0.000136
H	-5.861383	-2.414926	0.000238
H	-9.489108	-0.304264	0.000022
H	-8.552209	-2.640768	0.000196
H	6.617383	-1.866509	0.000261
H	7.858358	0.549289	0.000357
H	5.894829	2.410631	0.000229
H	-2.933406	2.760487	-0.000143

bdpsq-5-enPY6

C	-1.938791	2.010458	-0.000372
C	-2.213413	0.629625	-0.000069
C	-0.962799	-0.023198	0.000102
C	0.039164	0.953337	0.000003
N	-0.603561	2.188328	-0.000308
H	-0.106241	3.070631	-0.000394
H	-0.788977	-1.088383	0.000302
C	1.437495	0.902789	0.000049
C	2.452858	1.994137	-0.000195
C	2.485736	-0.054115	0.000169
C	3.517348	0.938727	-0.000009
O	2.387305	3.203059	-0.000470
O	2.603825	-1.325413	0.000319
C	4.848460	0.598999	-0.000123
C	6.093298	1.277807	-0.000047
N	5.098335	-0.787978	0.000138
C	7.075474	0.304322	0.000208
C	6.420998	-0.953110	0.000338
B	4.014822	-1.949723	0.000121
F	4.142208	-2.695399	1.149992
F	4.142010	-2.695054	-1.150027
C	-3.509258	-0.027034	-0.000037
C	-4.710043	0.580475	0.000007
H	-3.463575	-1.112075	-0.000008
H	-4.749824	1.667160	0.000159
C	-6.019152	-0.074185	-0.000018
C	-6.207673	-1.466219	-0.001069
C	-7.182476	0.709807	0.001040
C	-7.497666	-1.980294	-0.000913
H	-5.367888	-2.150298	-0.002093
C	-8.431100	0.095167	0.001091
H	-7.114618	1.792421	0.001849
N	-8.606399	-1.228694	0.000153
H	-7.652077	-3.055638	-0.001714
H	-9.334827	0.698337	0.001926
H	6.857525	-1.940988	0.000559

bdpsq-5-NMe2

C	-3.825807	1.395276	-0.073855
C	-3.911323	-0.014564	-0.112286
C	-2.587690	-0.498332	-0.091640
C	-1.726805	0.611478	-0.062202
N	-2.519483	1.747865	-0.052844
H	-2.143124	2.686534	-0.020865
H	-2.257440	-1.523576	-0.097177
C	-0.339026	0.745405	-0.032668
C	0.527839	1.960436	0.009291
C	0.831254	-0.063189	-0.027024
C	1.718530	1.054874	0.012183
O	0.303601	3.150878	0.030653
O	1.117371	-1.308721	-0.047885
C	3.087003	0.893341	0.030784
C	4.228462	1.728987	0.060438
N	3.516683	-0.446777	0.010784
C	5.333414	0.892337	0.057797
C	4.852523	-0.437227	0.027007
B	2.597639	-1.738059	-0.015201
F	2.794378	-2.468758	1.137443
F	2.849027	-2.461509	-1.161046
N	-5.080151	-0.754739	-0.191030
C	-4.984336	-2.173244	0.120697
H	-4.732747	-2.362650	1.175845
H	-5.939371	-2.650746	-0.100782
H	-4.225192	-2.646106	-0.505005
C	-6.319027	-0.095112	0.191623
H	-7.157335	-0.755706	-0.031624
H	-6.354430	0.164931	1.261416
H	-6.459656	0.817546	-0.392087
H	5.414125	-1.359468	0.016695
H	6.372779	1.180710	0.075242
H	4.210529	2.807443	0.079639
H	-4.604175	2.139293	-0.064253

H	8.144081	0.451670	0.000310
H	6.217867	2.349370	-0.000190
H	-2.611950	2.852742	-0.000590

bdpsq-5-PY5

C	-3.204110	1.824347	-0.047380
C	-3.405150	0.433548	-0.009652
C	-2.124016	-0.148667	0.007292
C	-1.173680	0.882672	-0.022217
N	-1.878566	2.081102	-0.052163
H	-1.431636	2.988454	-0.078596
H	-1.883875	-1.199433	0.052160
C	0.221926	0.898251	-0.018490
C	1.194288	2.031051	-0.041723
C	1.313294	-0.012372	0.002722
C	2.299165	1.021167	-0.016660
O	1.080315	3.236303	-0.069622
O	1.485201	-1.278558	0.030272
C	3.646495	0.737051	-0.005286
C	4.859678	1.466540	-0.011424
N	3.953302	-0.636704	0.024827
C	5.883688	0.534115	0.015209
C	5.283772	-0.747285	0.036796
B	2.920399	-1.840403	0.033931
F	3.079747	-2.576104	1.188040
F	3.077874	-2.591611	-1.111117
C	-4.699164	-0.237822	0.002833
C	-4.933345	-1.572500	-0.279997
C	-5.971782	0.345571	0.306801
N	-6.278765	-1.802319	-0.155047
H	-4.256585	-2.358904	-0.571551
C	-6.921300	-0.641399	0.201702
H	-6.163399	1.368638	0.590922
H	-6.727836	-2.689761	-0.309092
H	-7.987281	-0.615044	0.356911
H	5.759999	-1.716215	0.059677
H	6.945016	0.727202	0.019453
H	4.939364	2.542175	-0.031987
H	-3.928833	2.622214	-0.081537

bdpsq-5-PY6

C	-2.917380	1.946521	0.089320
C	-3.150060	0.564135	0.028779
C	-1.883658	-0.054622	0.004152
C	-0.911332	0.950666	0.046106
N	-1.586060	2.165455	0.099668
H	-1.115737	3.060469	0.150730
H	-1.672040	-1.110211	-0.062244
C	0.489001	0.931992	0.037801
C	1.481747	2.043031	0.080807
C	1.554972	-0.003009	-0.004631
C	2.567617	1.009335	0.032309
O	1.393837	3.248907	0.133520
O	1.697870	-1.270642	-0.057341
C	3.904284	0.696404	0.011965
C	5.136170	1.399360	0.030131
N	4.181377	-0.684546	-0.046089
C	6.136581	0.446655	-0.016948
C	5.506333	-0.823030	-0.062805
B	3.120273	-1.867467	-0.077462
F	3.264682	-2.641352	1.051535
F	3.260731	-2.577225	-1.247671
C	-4.465115	-0.089445	0.004726
C	-5.610971	0.570267	-0.459698
C	-4.633683	-1.408204	0.445944
C	-6.832187	-0.095912	-0.454325
H	-5.557230	1.582673	-0.842910
C	-5.898664	-1.985884	0.403214
H	-3.797486	-1.976756	0.834993
N	-6.992747	-1.354511	-0.034151
H	-7.726208	0.406357	-0.813221
H	-6.040213	-3.007656	0.743824
H	5.962366	-1.801158	-0.105807
H	7.202117	0.614732	-0.019519
H	5.239702	2.472347	0.071965
H	-3.618942	2.763258	0.148221

bdpsq-6-enNMe2

C	-2.886829	3.559743	0.025692
C	-3.515656	2.328088	0.047816
C	-2.514791	1.317893	0.034980
C	-1.262827	2.012625	0.008168
N	-1.545556	3.381153	0.001514
H	-0.828022	4.093086	-0.013569
C	0.052682	1.584498	-0.006681
C	1.336065	2.363314	-0.030583
C	0.831993	0.386020	-0.000351
C	2.075230	1.069041	-0.022628

bdpsq-6-enPY5

C	-1.496340	4.423501	-0.000355
C	-2.441203	3.411947	-0.000313
C	-1.757963	2.168704	-0.000204
C	-0.366884	2.486172	-0.000044
N	-0.258011	3.875720	-0.000130
H	0.630669	4.359238	-0.000145
C	0.790160	1.716899	0.000167
C	2.227443	2.139212	0.000283
C	1.226371	0.357926	0.000161
C	2.608874	0.696834	0.000361

O	1.591028	3.548055	-0.046249
O	0.617434	-0.879371	0.021443
C	3.280802	0.384958	-0.021036
C	4.651437	0.713995	-0.030817
N	3.158158	-1.014712	0.000373
C	5.351286	-0.488560	-0.015262
C	4.399200	-1.525653	0.003797
B	1.819812	-1.844108	0.009484
F	1.740776	-2.612994	1.156306
F	1.722432	-2.608060	-1.139385
C	-2.640358	-0.106657	0.039244
C	-3.837624	-0.763790	0.032463
H	-1.721883	-0.678680	0.041208
H	-4.763724	-0.199189	-0.014004
N	-4.018979	-2.106405	0.098516
C	-2.874323	-3.008544	0.120119
H	-3.215871	-4.008121	0.389160
H	-2.373506	-3.057046	-0.854768
H	-2.145660	-2.680675	0.863037
C	-5.313370	-2.685816	-0.226999
H	-5.347625	-3.049911	-1.262512
H	-5.527246	-3.524716	0.440045
H	-6.095560	-1.936620	-0.099613
H	4.558527	-2.593247	0.019072
H	6.421910	-0.621245	-0.016728
H	5.052124	1.715484	-0.046430
H	-3.318007	4.549032	0.027970
H	-4.583935	2.185216	0.075507

O	2.780971	3.217185	0.000290
O	0.693901	-0.807242	-0.000007
C	3.595163	-0.270544	0.000215
C	5.007383	-0.304729	0.000356
N	3.117337	-1.593095	-0.000028
C	5.373290	-1.643924	0.000168
C	4.183304	-2.402958	-0.000045
B	1.606214	-2.052118	-0.000281
F	1.330579	-2.766676	1.147888
F	1.330751	-2.766000	-1.148908
C	-2.287641	0.831486	-0.000152
C	-3.605235	0.515936	0.000110
H	-1.561018	0.026428	-0.000363
H	-4.339372	1.318568	0.000317
C	-4.144884	-0.820305	0.000132
C	-5.502679	-1.124271	0.000467
C	-3.445371	-2.076290	-0.000145
N	-5.633265	-2.482894	0.000363
H	-6.362476	-0.473351	0.000726
C	-4.383909	-3.072218	-0.000022
H	-2.376819	-2.222901	-0.000430
H	-6.508129	-2.980594	0.000437
H	-4.273625	-4.144215	-0.000174
H	4.064215	-3.476056	-0.000230
H	6.373288	-2.048588	0.000191
H	5.651628	0.560542	0.000555
H	-1.633724	5.493680	-0.000456
H	-3.508370	3.564012	-0.000384

bdpsq-6-enPY6

C	-0.897219	4.630352	0.000013
C	-1.930416	3.708151	-0.000021
C	-1.361238	2.410914	-0.000039
C	0.048535	2.597694	0.000000
N	0.284283	3.967111	-0.000021
H	1.213934	4.367484	0.000139
C	1.134683	1.721820	0.000028
C	2.602156	2.010367	0.000098
C	1.434637	0.331026	0.000006
C	2.847705	0.534482	-0.000042
O	3.255052	3.029520	0.000196
O	0.792115	-0.776124	-0.000076
C	3.733176	-0.519252	-0.000272
C	5.139021	-0.689920	-0.000580
N	3.130603	-1.792270	-0.000309
C	5.373448	-2.054425	-0.000986
C	4.112343	-2.697120	-0.000822
B	1.579234	-2.106680	0.000721
F	1.240233	-2.785118	1.150414
F	1.239343	-2.787168	-1.147537
C	-2.013635	1.122153	-0.000092
C	-3.349213	0.929860	-0.000101
H	-1.356543	0.259516	-0.000123

bdpsq-6-NMe2

C	-4.123562	1.945305	0.000134
C	-4.483610	0.609851	-0.000025
C	-3.290084	-0.163040	-0.000095
C	-2.188045	0.776347	0.000023
N	-2.786336	2.053610	0.000169
H	-2.224859	2.899882	0.000235
C	-0.799140	0.776813	-0.000044
C	0.076090	2.005430	0.000094
C	0.415370	-0.001715	-0.000092
C	1.265662	1.131560	0.000045
O	-0.166404	3.196666	0.000171
O	0.760681	-1.235089	-0.000264
C	2.647982	1.019406	-0.000018
C	3.749085	1.898324	-0.000241
N	3.128257	-0.298831	-0.000106
C	4.892712	1.104618	-0.000483
C	4.469497	-0.237543	-0.000381
B	2.261778	-1.610388	0.000307
F	2.495854	-2.339786	1.149665
F	2.496476	-2.340934	-1.148176
N	-3.254102	-1.515732	-0.000243
C	-4.516332	-2.244347	-0.000030
H	-5.111866	-2.008229	-0.888990

H	-4.006488	1.795716	-0.000075
C	-4.033797	-0.361334	-0.000148
C	-3.373878	-1.602054	-0.000146
C	-5.436756	-0.397260	-0.000211
C	-4.126041	-2.769771	-0.000195
H	-2.293074	-1.670884	-0.000104
C	-6.094697	-1.623184	-0.000259
H	-6.009908	0.523731	-0.000220
N	-5.465659	-2.801330	-0.000251
H	-3.626165	-3.733816	-0.000195
H	-7.180657	-1.659213	-0.000304
H	3.892919	-3.754519	-0.000957
H	6.329138	-2.554663	-0.001351
H	5.863168	0.109676	-0.000616
H	-0.933963	5.708405	0.000056
H	-2.979520	3.955797	-0.000032
H	-4.310354	-3.312332	0.000412
H	-5.111933	-2.007536	0.888692
C	-1.995026	-2.245758	-0.000547
H	-1.397379	-2.015165	0.884115
H	-2.201089	-3.314054	-0.001397
H	-1.397147	-2.013907	-0.884708
H	5.065003	-1.137908	-0.000472
H	5.918703	1.437985	-0.000707
H	3.688329	2.975394	-0.000266
H	-4.756646	2.819300	0.000224
H	-5.493151	0.237546	-0.000105

bdpsq-6-PY5

C	3.576717	-2.823946	0.025741
C	4.072898	-1.527714	0.056721
C	2.985143	-0.629576	-0.002641
C	1.806935	-1.438203	-0.048761
N	2.233454	-2.772801	-0.044242
H	1.581002	-3.549098	-0.065481
C	0.429033	-1.235187	-0.039802
C	-0.644859	-2.283877	-0.061384
C	-0.604246	-0.245560	0.014010
C	-1.659595	-1.200268	-0.013790
O	-0.624263	-3.496545	-0.097273
O	-0.704805	1.029927	0.073500
C	-2.988765	-0.825725	0.026335
C	-4.242515	-1.475670	0.057184
N	-3.205255	0.562359	0.075074
C	-5.206176	-0.478619	0.125172
C	-4.528211	0.759184	0.133367
B	-2.099806	1.683950	0.008007
F	-2.218163	2.531345	1.087382
F	-2.173101	2.351245	-1.202795
C	3.114434	0.812827	-0.010959
C	2.231968	1.752332	-0.527758
C	4.242526	1.547646	0.492538
N	2.777683	2.987119	-0.344140
H	1.271916	1.639040	-0.998324
C	4.001223	2.879418	0.281063
H	5.110613	1.135569	0.982166
H	2.333073	3.850399	-0.611538
H	4.583378	3.751942	0.527340
H	-4.938910	1.756711	0.177633
H	-6.276548	-0.605823	0.167796
H	-4.391559	-2.543921	0.037694
H	4.103479	-3.765492	0.038311
H	5.116289	-1.258573	0.084209

bdpsq-6-PY6

C	-3.264784	3.186390	0.025182
C	-3.834059	1.919072	0.064683
C	-2.796230	0.967583	-0.003661
C	-1.582589	1.699111	-0.067233
N	-1.925167	3.050259	-0.055579
H	-1.228135	3.787046	-0.079414
C	-0.214645	1.395023	-0.066664
C	0.932341	2.352343	-0.097369
C	0.719396	0.320360	0.003906
C	1.859122	1.186238	-0.031586
O	1.011602	3.561477	-0.141777
O	0.704423	-0.952843	0.092542
C	3.144256	0.703948	0.040536
C	4.453234	1.245118	0.096735
N	3.239312	-0.698662	0.120118
C	5.320223	0.173290	0.211591
C	4.533004	-1.005094	0.221441
B	2.037171	-1.727749	0.020260
F	2.083841	-2.595877	1.082641
F	2.073444	-2.359162	-1.206622
C	-2.985833	-0.489071	-0.021990
C	-3.963150	-1.087367	0.786707
C	-2.251745	-1.333138	-0.861766
C	-4.150726	-2.463144	0.719903
H	-4.553746	-0.492331	1.473303
C	-2.516043	-2.700377	-0.849278
H	-1.497147	-0.941589	-1.530827
N	-3.447748	-3.270951	-0.080900
H	-4.900549	-2.941363	1.343902
H	-1.948764	-3.366462	-1.492218
H	4.856055	-2.032984	0.295260
H	6.395945	0.205921	0.284924
H	4.694619	2.296041	0.064040
H	-3.732654	4.158076	0.039192
H	-4.890649	1.706446	0.097948

bdpsq-pristine

C	-4.983911	0.186130	-0.004646
C	-4.765006	-1.191626	-0.011578
C	-3.379761	-1.398268	-0.010283
C	-2.765141	-0.135721	-0.002498
N	-3.784322	0.810732	0.000778
H	-3.614903	1.808380	0.006310
H	-5.907455	0.742998	-0.003275
H	-5.534546	-1.946850	-0.016881
H	-2.854574	-2.340503	-0.014293
C	-1.428938	0.277132	0.002275
C	-0.823503	1.640609	0.008967
C	-0.125248	-0.285146	0.000107
C	0.525961	0.988642	0.005844
O	-1.277114	2.762824	0.013837
O	0.401081	-1.449058	-0.007448
C	1.895892	1.101391	0.000640
C	2.851271	2.148026	-0.005164
N	2.583417	-0.128619	-0.006993
C	4.097439	1.547302	-0.016589
H	2.620250	3.201784	-0.002459
C	3.888280	0.145836	-0.017234
H	5.059590	2.034997	-0.024077
B	1.936200	-1.579942	0.006536
F	2.291105	-2.228377	1.168585
F	2.311023	-2.258882	-1.130845
H	4.622077	-0.646522	-0.024317

ST8b : Optimised coordinates of systems with bdp2sq fusion scheme

bdp2sq-1-enNMe2

C	5.859668	0.790114	-0.012126
C	5.658407	2.178988	-0.019747
C	4.281008	2.399031	-0.019810
C	3.671880	1.132760	-0.012054
N	4.674007	0.151070	-0.007392
H	6.786105	0.236441	-0.009845
H	6.437118	2.925402	-0.024594
H	3.761679	3.344605	-0.024501
C	2.377725	0.622808	-0.006753
C	2.121692	-0.791646	0.004007
C	0.954056	0.821747	-0.003728
C	0.679350	-0.599674	0.007266
O	2.944576	-1.744504	0.009045
O	0.121277	1.772827	-0.006782
C	-0.596076	-1.091830	0.017857
C	-1.202229	-2.377658	0.034771
N	-1.615900	-0.120827	0.016181
C	-2.557719	-2.181387	0.043768
C	-2.810551	-0.762398	0.030975

bdp2sq-1-enPY5

C	6.305037	0.907734	-0.000043
C	6.063924	2.293071	-0.000017
C	4.683515	2.473505	0.000007
C	4.109766	1.188087	0.000046
N	5.141099	0.235233	-0.000017
H	7.247879	0.382194	-0.000051
H	6.821656	3.060723	-0.000035
H	4.136822	3.403522	0.000011
C	2.834389	0.642447	-0.000111
C	2.616885	-0.780358	-0.000108
C	1.402410	0.800988	-0.000031
C	1.172571	-0.626032	-0.000001
O	3.466229	-1.709361	-0.000193
O	0.544893	1.726725	-0.000033
C	-0.090159	-1.160222	-0.000032
C	-0.651936	-2.464240	-0.000068
N	-1.136805	-0.222477	-0.000039
C	-2.015008	-2.310048	-0.000063
C	-2.308508	-0.904319	-0.000091

B	-1.405226	1.440305	-0.007327
F	-1.929935	2.015614	1.130287
F	-1.920904	1.979904	-1.166064
B	4.490722	-1.406973	-0.000529
F	4.992651	-1.964855	-1.150878
F	5.005507	-1.956141	1.148157
H	-3.313665	-2.950637	0.062610
H	-0.668800	-3.315681	0.042049
C	-4.055147	-0.071248	0.030521
C	-5.261485	-0.716683	0.018256
H	-4.014578	1.008441	0.034527
H	-5.293274	-1.800150	-0.025376
N	-6.480072	-0.136602	0.069614
C	-6.613190	1.314282	0.103090
H	-6.355591	1.766224	-0.862351
H	-7.643840	1.570651	0.346940
H	-5.960352	1.736251	0.869761
C	-7.684441	-0.913783	-0.188620
H	-8.461294	-0.657269	0.536233
H	-8.074110	-0.727074	-1.196899
H	-7.463506	-1.977165	-0.095766

B	-0.977064	1.348978	-0.000062
F	-1.507105	1.886510	1.149217
F	-1.507030	1.886476	-1.149382
B	5.002107	-1.330362	0.000103
F	5.526328	-1.865434	-1.149550
F	5.525822	-1.865240	1.150058
C	-3.585052	-0.253342	-0.000033
C	-4.771038	-0.912137	0.000028
H	-3.574626	0.829273	-0.000056
H	-4.768170	-1.999139	0.000002
H	-0.088223	-3.384336	-0.000061
H	-2.750215	-3.098860	-0.000076
C	-6.071520	-0.299180	0.000020
C	-7.272633	-1.003533	-0.000092
C	-6.417289	1.096194	0.000191
N	-8.292828	-0.100390	-0.000004
H	-7.456510	-2.066111	-0.000268
C	-7.782491	1.183797	0.000205
H	-5.735120	1.931214	0.000303
H	-9.272299	-0.333728	-0.000052
H	-8.434970	2.041412	0.000372

bdp2sq-1-enPY6

C	6.535163	0.946507	0.000570
C	6.279257	2.333303	0.000640
C	4.900972	2.499261	0.000174
C	4.338951	1.204740	-0.000188
N	5.382480	0.262223	0.000017
H	7.484798	0.432868	0.000905
H	7.029966	3.107730	0.000992
H	4.344215	3.423291	0.000054
C	3.074415	0.647534	-0.000437
C	2.868931	-0.780541	-0.000168
C	1.637494	0.790663	-0.000207
C	1.426569	-0.635948	0.000050
O	3.726359	-1.700396	0.000063
O	0.772582	1.708016	-0.000198
C	0.165852	-1.187923	0.000264
C	-0.379610	-2.495647	0.000485
N	-0.886261	-0.261023	0.000201
C	-1.747446	-2.354326	0.000507
C	-2.049864	-0.956356	0.000316
B	-0.745419	1.315248	-0.000337
F	-1.282259	1.842542	1.148641
F	-1.281823	1.841766	-1.149825
B	5.260391	-1.308818	-0.000185
F	5.787566	-1.833060	-1.150658
F	5.788032	-1.833318	1.149970
C	-3.334988	-0.305900	0.000254
C	-4.514392	-0.963344	0.000078
H	-3.317348	0.776516	0.000364
H	-4.511627	-2.049785	-0.000099
C	-5.841587	-0.354656	0.000069

bdp2sq-1-NMe2

C	5.151870	0.764152	0.239263
C	4.957275	2.150098	0.337587
C	3.585029	2.384554	0.245975
C	2.972500	1.129723	0.093085
N	3.966905	0.140280	0.091692
H	6.072759	0.202011	0.266930
H	5.736465	2.885454	0.462553
H	3.071658	3.332522	0.286827
C	1.678028	0.632922	-0.027107
C	1.414304	-0.777513	-0.109558
C	0.257069	0.838384	-0.044485
C	-0.028966	-0.573558	-0.137823
O	2.228274	-1.736656	-0.110141
O	-0.580796	1.782658	0.040943
C	-1.299826	-1.065987	-0.114607
C	-1.859119	-2.363547	-0.015410
N	-2.347896	-0.105201	-0.068229
C	-3.211891	-2.213955	0.108894
H	-1.295536	-3.283666	-0.032426
C	-3.511235	-0.800519	0.063019
H	-3.942865	-3.001154	0.184595
B	-2.091986	1.459342	-0.117497
F	-2.733882	2.078723	0.929275
F	-2.437581	1.970183	-1.357920
B	3.780041	-1.405291	-0.091701
F	4.261879	-1.820372	-1.309398
F	4.303316	-2.092660	0.973514
N	-4.760908	-0.298762	0.134915
C	-5.166757	1.042624	-0.294612
H	-6.139202	0.957178	-0.784918

C	-6.976411	-1.179938	-0.000339
C	-6.070861	1.031478	0.000458
C	-8.244167	-0.606047	-0.000363
H	-6.871404	-2.259434	-0.000644
C	-7.377449	1.501901	0.000397
H	-5.252310	1.740453	0.000834
N	-8.459276	0.711851	-0.000006
H	-9.128691	-1.236637	-0.000682
H	-7.568706	2.570947	0.000694
H	0.192612	-3.410347	0.000608
H	-2.475113	-3.150021	0.000652

H	-5.249974	1.723309	0.555752
H	-4.460812	1.452976	-1.008424
C	-5.857156	-1.170175	0.557395
H	-6.626589	-0.552673	1.021951
H	-6.304672	-1.702887	-0.290209
H	-5.518378	-1.891650	1.299370

bdp2sq-1-PY5

C	-5.556393	-0.858307	-0.115785
C	-5.329456	-2.245421	-0.164470
C	-3.952012	-2.441543	-0.125958
C	-3.365522	-1.163770	-0.054233
N	-4.386734	-0.199823	-0.049330
H	-6.493421	-0.322522	-0.125532
H	-6.094505	-3.003609	-0.221674
H	-3.415130	-3.377020	-0.147425
C	-2.085529	-0.632722	0.001084
C	-1.853383	0.787025	0.046645
C	-0.655183	-0.805020	0.014368
C	-0.410568	0.616011	0.063797
O	-2.692304	1.725274	0.052119
O	0.197912	-1.732891	-0.018914
C	0.853466	1.143230	0.068229
C	1.396988	2.450812	0.052963
N	1.912141	0.207841	0.047696
C	2.759888	2.308585	0.017872
C	3.072150	0.907865	0.016071
B	1.721498	-1.365886	0.048431
F	2.170647	-1.905058	1.234099
F	2.290942	-1.922586	-1.067512
B	-4.232446	1.362363	0.034692
F	-4.753911	1.962732	-1.082696
F	-4.747204	1.839751	1.213784
C	4.413850	0.376415	-0.011718
C	5.526914	1.162583	-0.316440
C	4.909825	-0.946044	0.251378
N	6.630055	0.374040	-0.247447
H	5.598995	2.200691	-0.594897
C	6.268387	-0.913050	0.101472
H	4.330520	-1.805899	0.534793
H	7.570057	0.681621	-0.437215
H	7.007772	-1.688135	0.216472
H	0.822297	3.363839	0.070063
H	3.490254	3.101727	0.016994

bdp2sq-1-PY6

C	-5.733234	-0.891046	0.308184
C	-5.483778	-2.272568	0.457631
C	-4.112018	-2.456340	0.369801
C	-3.545762	-1.178112	0.167717
N	-4.583090	-0.228130	0.134019
H	-6.678159	-0.368726	0.319757
H	-6.235578	-3.030264	0.612452
H	-3.560474	-3.380666	0.442327
C	-2.283500	-0.640011	0.022660
C	-2.069227	0.780457	-0.122004
C	-0.846429	-0.794483	-0.013580
C	-0.630080	0.621292	-0.159382
O	-2.920068	1.705837	-0.158435
O	0.017155	-1.706158	0.075182
C	0.631553	1.174245	-0.183295
C	1.152682	2.485737	-0.161371
N	1.695841	0.253250	-0.115829
C	2.521866	2.360143	-0.060994
C	2.840763	0.972874	-0.040328
B	1.528944	-1.326005	-0.142258
F	2.220829	-1.904829	0.880895
F	1.836864	-1.815305	-1.394031
B	-4.455385	1.326165	-0.102732
F	-4.975376	1.671004	-1.322472
F	-4.986558	2.016093	0.952692
H	0.568153	3.391456	-0.206829
H	3.248960	3.156148	-0.035161
C	4.207473	0.437914	0.040000
C	5.148544	1.100142	0.842349
C	4.650449	-0.676223	-0.682528
C	6.453650	0.623124	0.891294
H	4.865194	1.957948	1.440065
C	5.982501	-1.063680	-0.565589
H	3.984954	-1.225881	-1.332552
N	6.880492	-0.438958	0.201724
H	7.190870	1.117906	1.516964
H	6.344331	-1.922763	-1.122586

bdp2sq-2-enNMe2

bdp2sq-2-enPY5

C	5.717104	-0.985077	0.009248
C	6.185602	0.341711	-0.017884
C	5.071330	1.174205	-0.032598
C	3.940701	0.333944	-0.013871
N	4.374085	-1.002132	0.011857
H	6.282499	-1.904486	0.026343
H	7.222235	0.639613	-0.025265
H	5.049824	2.252584	-0.053330
C	2.563325	0.482116	-0.010854
C	1.676025	-0.651550	0.019167
C	1.391165	1.322615	-0.019703
C	0.493849	0.189729	0.011589
O	1.962192	-1.877411	0.043517
O	1.106438	2.551383	-0.041883
C	-0.874747	0.330347	0.026458
C	-2.009718	-0.502028	0.076009
N	-1.301826	1.676393	0.006046
C	-3.136888	0.326086	0.079096
C	-2.631448	1.662943	0.038661
B	-0.402825	2.975053	-0.059030
F	-0.611131	3.748307	1.054435
F	-0.612672	3.636022	-1.243174
B	3.485237	-2.299632	0.032585
F	3.669446	-3.032261	-1.112927
F	3.693370	-3.011568	1.186543
H	-1.975890	-1.579188	0.120363
C	-4.549081	0.019236	0.107790
C	-5.053362	-1.238741	0.009826
H	-5.219363	0.864657	0.208609
H	-4.375637	-2.072075	-0.150473
N	-6.361131	-1.617350	0.116113
C	-7.394985	-0.611260	0.281168
H	-7.546038	-0.016106	-0.631125
H	-8.335145	-1.102271	0.534413
H	-7.131300	0.066017	1.096445
C	-6.775212	-2.900192	-0.434427
H	-7.612076	-3.299394	0.143208
H	-7.085415	-2.820011	-1.485836
H	-5.948621	-3.609476	-0.373974
H	-3.197145	2.583879	0.029723

C	6.114175	-1.305463	-0.001215
C	6.678718	-0.014133	-0.001089
C	5.629320	0.896009	-0.000100
C	4.439220	0.138879	0.000385
N	4.775334	-1.226085	-0.000338
H	6.612389	-2.263221	-0.001878
H	7.734357	0.207182	-0.001663
H	5.685768	1.973326	0.000242
C	3.078703	0.385829	0.000590
C	2.109721	-0.681162	-0.000086
C	1.969308	1.310736	0.000565
C	0.994690	0.244680	-0.000051
O	2.305732	-1.924490	-0.000557
O	1.775211	2.555897	0.000984
C	-0.361769	0.485629	-0.000179
C	-1.551196	-0.265888	-0.000383
N	-0.692517	1.858258	0.000334
C	-2.616006	0.640725	0.000037
C	-2.021355	1.938060	0.000447
B	0.296816	3.090794	-0.000091
F	0.143667	3.821295	1.149609
F	0.144883	3.819598	-1.151036
B	3.793244	-2.457655	0.000442
F	3.938553	-3.190801	-1.148848
F	3.937594	-3.188604	1.151321
C	-4.047205	0.420082	0.000131
C	-4.655502	-0.785320	-0.000251
H	-4.658372	1.318201	0.000528
H	-4.035959	-1.679556	-0.000692
H	-1.597857	-1.343408	-0.000661
C	-6.080709	-1.024977	-0.000190
C	-6.664133	-2.285959	-0.000607
C	-7.161486	-0.078923	0.000333
N	-8.021836	-2.128726	-0.000303
H	-6.208793	-3.263437	-0.000993
C	-8.335122	-0.786057	0.000197
H	-7.081702	0.996509	0.000817
H	-8.691614	-2.880053	-0.000668
H	-9.359977	-0.452664	0.000497
H	-2.521467	2.896173	0.000833

bdp2sq-2-enPY6

C	6.322647	-1.411440	0.000456
C	6.921461	-0.131834	0.000714
C	5.898023	0.802663	0.000625
C	4.686438	0.074585	0.000286
N	4.989260	-1.299950	0.000227
H	6.798442	-2.380760	0.000427
H	7.982564	0.061388	0.000914
H	5.981265	1.878255	0.000783
C	3.336757	0.354567	0.000049
C	2.337849	-0.688280	-0.000229
C	2.248438	1.309048	0.000036

bdp2sq-2-NMe2

C	5.216365	-0.041968	-0.020221
C	5.364995	1.357733	-0.034291
C	4.088564	1.909692	-0.034805
C	3.183086	0.830256	-0.020782
N	3.914151	-0.369526	-0.012106
H	5.979459	-0.805511	-0.016018
H	6.304530	1.887437	-0.042505
H	3.818050	2.953994	-0.042722
C	1.809178	0.655574	-0.007432
C	1.208324	-0.653097	0.018075
C	0.475092	1.202008	0.003212

C	1.251552	0.266877	-0.000275
O	2.501311	-1.935437	-0.000294
O	2.086482	2.557347	0.000223
C	-0.101817	0.544107	-0.000255
C	-1.305158	-0.180466	-0.000250
N	-0.399905	1.921927	-0.000055
C	-2.347875	0.753492	0.000015
C	-1.727943	2.034905	0.000167
B	0.618547	3.131830	-0.000193
F	0.486055	3.862139	1.150148
F	0.486513	3.861456	-1.151060
B	3.974667	-2.509480	-0.000213
F	4.102243	-3.240061	-1.150913
F	4.101891	-3.240659	1.150130
C	-3.784482	0.557843	0.000118
C	-4.415033	-0.632269	0.000001
H	-4.372153	1.471308	0.000294
H	-3.816073	-1.539480	-0.000177
H	-2.204728	3.004702	0.000361
C	-5.860651	-0.854824	0.000073
C	-6.355244	-2.167648	-0.000004
C	-6.819189	0.172251	0.000216
C	-7.729412	-2.388303	0.000066
H	-5.673241	-3.011003	-0.000117
C	-8.168749	-0.154562	0.000274
H	-6.529490	1.215947	0.000279
N	-8.637634	-1.409257	0.000202
H	-8.118071	-3.402814	0.000004
H	-8.917133	0.632870	0.000384
H	-1.377822	-1.256602	-0.000433

C	-0.136520	-0.107090	0.029239
O	1.769692	-1.779358	0.027483
O	-0.086321	2.332414	-0.002314
C	-1.499796	-0.286607	0.054920
C	-2.409711	-1.364296	0.074602
N	-2.223048	0.920720	0.051170
C	-3.692978	-0.810074	0.097493
H	-2.133632	-2.405258	0.070314
C	-3.518582	0.611629	0.073637
B	-1.648638	2.395509	0.009710
F	-2.013619	3.072224	1.145470
F	-2.032465	3.013518	-1.153776
B	3.350326	-1.838128	-0.006438
F	3.681134	-2.489341	-1.167496
F	3.732858	-2.499801	1.131851
N	-4.903059	-1.462643	0.169518
C	-4.893994	-2.904590	-0.020004
H	-5.883803	-3.300995	0.206954
H	-4.626632	-3.193897	-1.047676
H	-4.181847	-3.368324	0.665828
C	-6.109946	-0.755221	-0.238738
H	-6.155042	-0.583537	-1.324155
H	-6.980005	-1.342522	0.055942
H	-6.179827	0.207661	0.269675
H	-4.268601	1.386651	0.072715

bdp2sq-2-PY5

C	5.619514	-0.468164	-0.034082
C	5.913597	0.910168	-0.037092
C	4.703059	1.591294	-0.024479
C	3.689166	0.610923	-0.014017
N	4.292154	-0.658967	-0.020273
H	6.299808	-1.306423	-0.040967
H	6.903358	1.338670	-0.047535
H	4.542204	2.658038	-0.023226
C	2.306755	0.579931	-0.002274
C	1.571643	-0.659437	0.001620
C	1.034985	1.264097	0.007800
C	0.293434	0.024172	0.010167
O	2.012605	-1.838368	-0.003094
O	0.594473	2.444660	0.011936
C	-1.082526	-0.010211	0.012990
C	-2.100468	-0.985097	-0.001454
N	-1.683010	1.265312	0.014564
C	-3.321359	-0.311974	-0.005740
C	-3.002318	1.077754	0.004105
B	-0.962012	2.671107	0.042290
F	-1.237695	3.323128	1.216311

bdp2sq-2-PY6

C	5.809361	-0.609097	-0.108993
C	6.153257	0.761539	-0.118236
C	4.971491	1.483626	-0.076172
C	3.921317	0.537740	-0.042036
N	4.480389	-0.754009	-0.063583
H	6.460987	-1.469818	-0.132646
H	7.157528	1.153380	-0.152410
H	4.848204	2.555362	-0.070970
C	2.544027	0.555213	-0.002296
C	1.761992	-0.658976	0.009411
C	1.294222	1.285105	0.028199
C	0.514277	0.072067	0.036976
O	2.159556	-1.852055	-0.007563
O	0.896723	2.479362	0.038037
C	-0.866628	0.088773	0.045469
C	-1.913766	-0.850776	0.020584
N	-1.422652	1.381502	0.050577
C	-3.110262	-0.132408	0.004662
C	-2.749279	1.242309	0.024067
B	-0.652845	2.761262	0.122454
F	-0.868496	3.363132	1.333544

F	-1.276698	3.386844	-1.083104
B	3.577185	-2.062558	-0.008064
F	3.861344	-2.758314	-1.154409
F	3.869780	-2.742795	1.145746
H	-3.679180	1.919019	0.011464
C	-4.668291	-0.857824	-0.013903
C	-5.023007	-2.183942	0.179835
C	-5.888555	-0.134652	-0.223251
N	-6.385462	-2.273753	0.092379
H	-4.417737	-3.052090	0.383204
C	-6.924077	-1.032357	-0.153039
H	-5.990752	0.921493	-0.417194
H	-6.914445	-3.123284	0.201302
H	-7.987198	-0.893711	-0.259926
H	-1.934192	-2.050798	-0.019699

F	-0.971241	3.535769	-0.959222
B	3.715431	-2.135106	-0.027264
F	3.963160	-2.848000	-1.168671
F	3.996792	-2.806804	1.131989
H	-1.786584	-1.921465	-0.011271
C	-4.478988	-0.660271	-0.023738
C	-4.775708	-1.951075	0.433885
C	-5.551264	0.098228	-0.512489
C	-6.087848	-2.408902	0.379322
H	-4.002273	-2.588182	0.846016
C	-6.829008	-0.452748	-0.519013
H	-5.399510	1.097259	-0.903723
N	-7.111249	-1.684697	-0.085154
H	-6.329959	-3.407144	0.732711
H	-7.667232	0.125270	-0.897504
H	-3.394812	2.107587	0.040805

bdp2sq-3-enNMe2

C	-4.802205	-0.252192	-0.053561
C	-5.058044	-1.630514	-0.092315
C	-3.824818	-2.282910	-0.082045
C	-2.840522	-1.282321	-0.037126
N	-3.473065	-0.029229	-0.020178
H	-5.501221	0.570109	-0.047874
H	-6.035165	-2.086186	-0.123940
H	-3.637863	-3.345155	-0.104180
C	-1.450366	-1.221686	-0.010456
C	-0.748163	0.021861	0.022609
C	-0.169560	-1.880104	-0.014209
C	0.560195	-0.618921	0.015402
O	-1.225359	1.194802	0.040248
O	0.287574	-3.051322	-0.043213
C	1.926701	-0.567069	-0.010138
C	2.970169	0.440510	-0.054584
N	2.538319	-1.843099	-0.048614
C	4.172300	-0.289911	-0.123593
C	3.864526	-1.648472	-0.116512
B	1.849284	-3.244885	0.060979
F	2.074753	-3.809059	1.294989
F	2.217480	-4.049514	-0.986940
B	-2.797394	1.377652	0.036139
F	-3.082603	2.118948	-1.087195
F	-3.098242	2.035570	1.206168
C	2.898292	1.865236	-0.046352
C	1.752858	2.615626	0.019927
H	3.856596	2.368459	-0.099513
H	0.783013	2.138222	0.050202
N	1.679802	3.961710	0.061265
C	2.879628	4.782821	0.013251
H	3.367762	4.725438	-0.967317
H	2.609413	5.820156	0.206602
H	3.594173	4.463903	0.776972
C	0.389548	4.640933	-0.015549

bdp2sq-3-enPY5

C	4.001787	-3.328288	-0.000070
C	5.194347	-2.580567	-0.000155
C	4.839899	-1.235830	-0.000189
C	3.431840	-1.190434	-0.000188
N	2.939619	-2.506674	-0.000115
H	3.872800	-4.400058	-0.000017
H	6.191342	-2.992115	-0.000165
H	5.493946	-0.377902	-0.000272
C	2.445900	-0.217359	-0.000091
C	1.047631	-0.553462	0.000001
C	2.051245	1.172497	-0.000022
C	0.642803	0.838518	0.000084
O	0.507045	-1.692651	0.000003
O	2.584096	2.312801	-0.000133
C	-0.332007	1.803011	-0.000062
C	-1.764631	1.821439	-0.000152
N	0.149568	3.121873	-0.000186
C	-2.111338	3.183974	-0.000341
C	-0.927406	3.927740	-0.000375
B	1.648948	3.590974	0.000194
F	1.943054	4.278328	1.150201
F	1.943304	4.279242	-1.149186
B	1.436741	-2.970119	0.000035
F	1.140094	-3.658774	-1.149270
F	1.140236	-3.658486	1.149581
C	-2.577751	0.636788	-0.000065
C	-3.933073	0.620715	-0.000089
H	-2.045137	-0.309661	0.000020
H	-4.464340	1.569702	-0.000180
C	-4.762656	-0.555630	-0.000023
C	-6.154526	-0.536505	-0.000024
C	-4.374620	-1.939994	0.000086
N	-6.596384	-1.826460	0.000084
H	-6.839098	0.296681	-0.000090
C	-5.518760	-2.690593	0.000135

H	0.295557	5.367481	0.796376
H	0.280671	5.167513	-0.970318
H	-0.415764	3.913719	0.071724
H	4.539469	-2.491098	-0.155101
H	5.165064	0.129257	-0.174497

H	-3.370178	-2.332508	0.000106
H	-7.563239	-2.107188	0.000023
H	-5.661524	-3.758719	0.000283
H	-0.809909	5.001462	-0.000517
H	-3.104164	3.604747	-0.000476

bdp2sq-3-enPY6

C	-2.459988	4.354275	0.000534
C	-3.849787	4.116203	0.000807
C	-4.033593	2.740342	0.000606
C	-2.746773	2.161284	0.000220
N	-1.790605	3.192579	0.000182
H	-1.934211	5.297270	0.000571
H	-4.614416	4.876839	0.001120
H	-4.964773	2.195613	0.000733
C	-2.209770	0.888100	0.000070
C	-0.791790	0.654430	-0.000092
C	-2.385203	-0.544326	0.000056
C	-0.955777	-0.789354	-0.000063
O	0.140123	1.504269	-0.000158
O	-3.332422	-1.370963	0.000176
C	-0.433692	-2.064853	0.000040
C	0.856028	-2.700636	0.000234
N	-1.421769	-3.070829	0.000173
C	0.590117	-4.075902	0.000489
C	-0.798057	-4.255638	0.000445
B	-2.989875	-2.904763	-0.000298
F	-3.524151	-3.424578	1.149379
F	-3.523375	-3.423609	-1.150795
B	-0.225810	3.046369	-0.000413
F	0.313767	3.561402	-1.149878
F	0.314693	3.562039	1.148324
C	2.190691	-2.147736	0.000235
C	2.547574	-0.847047	0.000033
H	2.969833	-2.904322	0.000432
H	1.784395	-0.078219	-0.000146
H	-1.362016	-5.176492	0.000584
H	1.326134	-4.865003	0.000701
C	3.914634	-0.326995	0.000048
C	4.113585	1.061938	-0.000056
C	5.068827	-1.128116	0.000148
C	5.409989	1.569512	-0.000046
H	3.266616	1.738486	-0.000140
C	6.317278	-0.520695	0.000145
H	5.008430	-2.209606	0.000224
N	6.505514	0.805510	0.000051
H	5.573441	2.643243	-0.000112
H	7.217242	-1.129114	0.000210

bdp2sq-3-NMe2

C	-4.776376	-0.333280	-0.134065
C	-4.858772	-1.732225	-0.221169
C	-3.556215	-2.227441	-0.192367
C	-2.705116	-1.113716	-0.088006
N	-3.488463	0.050011	-0.053719
H	-5.572229	0.395784	-0.125011
H	-5.770933	-2.302945	-0.296180
H	-3.238055	-3.257131	-0.240903
C	-1.336235	-0.882247	-0.023302
C	-0.791095	0.438037	0.054748
C	0.010345	-1.383683	-0.021265
C	0.588176	-0.046449	0.051223
O	-1.407044	1.538885	0.091105
O	0.596402	-2.497076	-0.078792
C	1.945505	0.146524	0.019686
C	2.889866	1.246614	-0.055759
N	2.689162	-1.054943	-0.076974
C	4.159768	0.656392	-0.226633
C	3.979205	-0.724105	-0.224446
B	2.155285	-2.512663	0.117010
F	2.364479	-2.947335	1.407121
F	2.678795	-3.344911	-0.837395
B	-2.991269	1.529135	0.076224
F	-3.360967	2.272987	-1.017126
F	-3.378708	2.079771	1.273448
N	2.623171	2.568560	0.014168
C	1.264940	3.062018	0.193280
H	1.297963	4.125518	0.421939
H	0.652851	2.921264	-0.703076
H	0.777326	2.555696	1.028472
C	3.716895	3.510470	-0.194468
H	4.139600	3.412763	-1.200719
H	3.342788	4.524704	-0.072941
H	4.515869	3.346626	0.535521
H	4.731720	-1.493334	-0.318645
H	5.103343	1.162738	-0.336643

bdp2sq-3-PY5

C	4.903921	-0.374216	-0.078701
C	5.281986	0.979801	-0.129791

bdp2sq-3-PY6

C	4.879360	-0.871654	-0.250413
C	5.430840	0.425883	-0.337698

C	4.114939	1.736809	-0.113207
C	3.043939	0.824676	-0.052316
N	3.565156	-0.479826	-0.032180
H	5.529379	-1.254019	-0.073113
H	6.295684	1.345566	-0.173886
H	4.021454	2.811159	-0.142360
C	1.659702	0.885934	-0.017423
C	0.844891	-0.292900	0.024293
C	0.442670	1.657888	-0.015933
C	-0.394024	0.469973	0.020837
O	1.215743	-1.500336	0.046501
O	0.098254	2.867046	-0.044489
C	-1.765148	0.544307	0.004670
C	-2.888502	-0.356312	-0.033034
N	-2.253213	1.870893	-0.033316
C	-4.016842	0.469205	-0.098087
C	-3.587677	1.801877	-0.095110
B	-1.435158	3.208329	0.062266
F	-1.607012	3.796748	1.291508
F	-1.732901	4.029827	-0.992962
B	2.765684	-1.826411	0.050634
F	2.991975	-2.603036	-1.057397
F	3.008828	-2.473605	1.236637
H	-4.184661	2.701311	-0.131526
H	-5.045369	0.149684	-0.141657
C	-2.899386	-1.800879	-0.020092
C	-1.819509	-2.671331	0.093976
C	-4.074309	-2.623693	-0.120851
N	-2.302301	-3.944130	0.063972
H	-0.762463	-2.490316	0.189324
C	-3.674898	-3.931466	-0.067021
H	-5.092375	-2.284738	-0.224985
H	-1.730616	-4.771254	0.126033
H	-4.241668	-4.846664	-0.111099

C	4.380712	1.327072	-0.256619
C	3.200897	0.560828	-0.121992
N	3.549192	-0.802347	-0.121307
H	5.385331	-1.825245	-0.274539
H	6.479257	0.653024	-0.449443
H	4.426228	2.404284	-0.294056
C	1.845489	0.797088	-0.028940
C	0.881743	-0.274379	0.032251
C	0.732903	1.718663	0.000255
C	-0.237590	0.647762	0.059372
O	1.089869	-1.515292	0.035747
O	0.540618	2.961703	-0.033512
C	-1.596708	0.896601	0.050597
C	-2.803856	0.141194	-0.036348
N	-1.918008	2.264354	-0.015260
C	-3.828079	1.081137	-0.167699
C	-3.247382	2.359451	-0.143948
B	-0.935652	3.487815	0.132143
F	-1.008621	4.012797	1.397761
F	-1.153636	4.393911	-0.868061
B	2.583774	-2.034799	0.067736
F	2.717698	-2.911263	-0.972056
F	2.756806	-2.595244	1.307598
C	-2.947777	-1.317937	-0.009550
C	-3.950820	-1.951239	-0.757729
C	-2.121989	-2.137657	0.769077
C	-4.074793	-3.334406	-0.693183
H	-4.610370	-1.378009	-1.398169
C	-2.327822	-3.514706	0.758808
H	-1.344598	-1.720866	1.396179
N	-3.284022	-4.118035	0.047559
H	-4.844567	-3.839355	-1.269732
H	-1.692643	-4.161612	1.356332
H	-3.729808	3.323520	-0.204533
H	-4.884442	0.876062	-0.240869

bdp2sq-pristine

C	4.294467	-0.869885	-0.000380
C	4.060673	-2.262667	-0.000568
C	2.687117	-2.450520	-0.000186
C	2.103821	-1.163640	-0.000057
N	3.133407	-0.204324	-0.000251
H	5.236452	-0.342094	-0.000496
H	4.824130	-3.024514	-0.000829
H	2.144714	-3.383075	-0.000126
C	0.833328	-0.627325	0.000097
C	0.603651	0.797515	-0.000014
C	-0.603651	-0.796435	0.000155
C	-0.833569	0.628279	0.000040
O	1.446608	1.731531	-0.000174
O	-1.446450	-1.730811	0.000208
C	-2.104108	1.164447	-0.000098
C	-2.688426	2.450732	-0.000355

N	-3.133168	0.204140	-0.000034
C	-4.061811	2.261953	-0.000506
C	-4.294754	0.868980	-0.000337
B	-2.983607	-1.367776	0.000378
F	-3.504893	-1.897436	-1.149805
F	-3.504460	-1.896802	1.151062
B	2.984969	1.367185	0.000034
F	3.505166	1.896432	1.150735
F	3.505647	1.896899	-1.150222
H	-2.147059	3.383900	-0.000443
H	-4.825421	3.023640	-0.000729
H	-5.236132	0.340187	-0.000384