Electronic Supplementary information

Mechanism Behind the Photochromism and Photomagnetism of Biindenilidenediones type II: Multiconfigurational, Perturbative and Density Functional Theory Studies

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Section I: Gas phase





Criteria for the definition of the active space:

Based on the hydrogen migration involved in the Norrish type II reaction, we can classify the PES in the FC zone, TS zone and Product zone. In order to keep an active space with reasonable size that allow calculation times accessible, instead of increasing the active space, we have chosen the most important molecular orbitals to describe the electronic nature of the excited states depending on the zone of the PES that we were exploring. We have used an active space (14,12) in all the calculations. However, they also were adapted to the PES zone according to Figure S3.



Figure S2. The active spaces used to study the hydrogen migration on BID-II derivatives

Initially, to study the transition state zone we included the π and π^* of the carbonyl group obtaining a CAS(16,14). We also tried with the CAS(14,12) as shown in Figure S3b, which lead to the same qualitatively results for the target states, so we decided to use the last active space mentioned in order to decrease the computation time.

The ideal situation would be to calculate the whole stationary points using CAS(16,14) such as in the transition state zone. Nevertheless, the molecular symmetry in the Franck-Condon geometry compels to include also the *n* on the other carbonyl plus the σ , σ^* and P_0 orbitals of the other HO group. This leads to an increase of the active space to (22,18) which is unaffordable with computation tools currently available in our group.

DDCI Space

This space was defined based in computational affordability and similar size of the configuration space in Model 1 and 2. Once it was confirmed that all relevant valence MO were included, we additionally included the maximum number of empty MO as long as the CPU time was accessible.



Figure S3. The electronic density differences between ground state and: (a) $(Ag)\ln\pi^*$, (b) $(Au)\ln\pi^*$ and (c) $(Au)\ln\pi^*$ at Franck-Condon geometry. Negative and positive differences are shown in red and blue, respectively.

		ΔΔΕ(Β2	B2-Mod)	
Irred. Rep.	Nature	ΔΔΕ (CASSCF)	ΔΔΕ (MS-CASPT2)	ΔΔΕ (IDDCI+DC)
	$^{3}n\pi^{*}$	-2.1 T ₂	+4.7 T ₁	+6.4 T ₁
Ag	$^{1}n\pi^{*}$	-1.8 S ₁	+1.7 S ₁	+6.8 S ₁
	$^{3}\pi\pi^{*}$	-5.5 T ₁	+1.8 T ₂	+3.6 T ₂
A _u	$^{1}\pi\pi^{*}$	-2.0 S ₅	+11.9 S ₃	+3.4 S ₂
	$^{3}n\pi^{*}$	-4.2 T ₃	+3.2 T ₃	+6.8 T ₃
Au	$^{1}n\pi^{*}$	-3.1 S ₂	+0.1 S ₂	+6.5 S ₃

Table S1. Excitation energy differences between Model-2 and Model-1 for the lower singlet and triplet states at FC geometry.



^a Energies calculated at SA3-CASSCF(14,12) level. ^b C=O distances (in Å) along symmetrical stretching.

Figure S4. The S_1 - S_2 energy gap in kcal·mol⁻¹ at the SA3-CASSCF(14,12) level in B2-Mod.



Figure S5. Contour diagrams calculated at CASSCF(14,12) level for the S₀, S₁ and S₂ PES for Model-1. RC1 and RC2 are the linear direction from FC to both mirror-image Min- $n\pi^*(S_1)$. M_i means minimum on the S_i.

Figure S6 shows all the stationary points located around the FC geometry on the S_1 and T_1 PESs. The 3*N*-6 dimensional nuclear configuration space is projected into a 2D space formed by the two carbonyl distances.



Figure S6. Stationary point located at CASSCF(14,12) on S_1 and T_1 in Model-1.



Figure S7. Graphical representation of the strategy used to get energy profiles at IDDCI+DC level. CP*i* means critical point *i*.



Figure S8. The spin density for the triplet states on the FC (first row), $LM^{-1}n\pi^*(S_1)$ (second row) and ${}^{3}P(p_0\pi^*)$ (third row).



Figure 57. Wis-CASI 12 chergy prome along the coordinate connecting $EW-m_{k}$ (1) and 1 (p_{0m})	Figure S9. MS-CASPT2	energy profile along the	coordinate connecting	LM- ³ $n\pi^*(T_1)$ and ³ P($p_0\pi$	*).
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zmat	ang	gstrom	S								
С											
С	1	cc2									
С	2	cc3	1	ccc3							
С	3	cc4	2	ccc4		1	dih4				
С	4	cc5	3	ccc5		2	dih5				
С	2	cc6	3	сссб		4	dih6				
0	2	oc7	3	occ7		4	dih7				
0	5	oc8	4	occ8		3	dih8				
С	1	cc9	2	ccc9		6	dih9				
С	9	cc10	1	ccc10		2	dih10				
С	10	cc11	9	ccc11		1	dih11				
С	11	cc12	10	ccc12		9	dih12				
С	12	cc13	11	ccc13		10	dih13				
С	10	cc14	9	ccc14		13	dih14				
0	10	oc15	9	occ15		13	dih15				
0	13	oc16	9	occ16		10	dih16				
vari	able	es:									
		For	$^{3}P(p_{0}\pi^{*})$			F	or the S_0 -FC		D	ifferences	
cc2			1.533364		CC2		1 5/3617		-2	0 010252	
cc3					002		1.04001/		22	-0.010233	
			1.514532		cc3		1.514452	cc	23	0.000080	
ccc	3		1.514532 103.425		cc3 ccc3		1.514452 102.091		23 203	0.000080	
ccc cc4	3		1.514532 103.425 1.337265		cc3 cc2 cc3 cc4		1.514452 102.091 1.338301		22 23 203 24	-0.010233 0.000080 1.334 -0.001036	
ccc cc4 ccc	3 4		1.514532 103.425 1.337265 112.237		cc3 ccc3 cc4 ccc4		1.514452 102.091 1.338301 113.698		22 23 203 24 204	-0.0010233 0.000080 1.334 -0.001036 -1.461	
ccc cc4 ccc dih	3 4 4		1.514532 103.425 1.337265 112.237 -6.464		cc3 ccc3 cc4 ccc4 dih4		1.514452 102.091 1.338301 113.698 -6.645	cc cc cc di	22 23 223 24 224 224 224	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181	
ccc cc4 ccc dih cc5	3 4 4		1.514532 103.425 1.337265 112.237 -6.464 1.481690		cc3 ccc3 ccc4 ccc4 dih4 cc5		1.514452 102.091 1.338301 113.698 -6.645 1.473990	cc cc cc di cc	22 23 24 24 204 204 25	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700	
ccc cc4 ccc dih cc5 ccc	3 4 4 5		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877		cc3 ccc3 ccc4 ccc4 dih4 cc5 ccc5		1.514452 102.091 1.338301 113.698 -6.645 1.473990 109.740	cc cc cc di cc cc	22 23 223 24 224 224 224 224 25 225	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137	
ccc cc4 ccc dih cc5 ccc dih	3 4 4 5 5		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5		1.514452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751	cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 223 24 224 224 224 224 225 225 245 225 245	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127	
ccc cc4 ccc dih cc5 ccc dih cc6	3 4 4 5 5		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6		1.54452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621	cc cc cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 24 24 24 25 25 25 26 25 26	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc	3 4 4 5 5 6		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6		1.54452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773	di cc di cc di cc	22 23 24 24 25 25 25 25 25 25 26 20 5 26 20 6	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih	3 4 5 5 6 6		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6 dih6		1.54452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804	di cc di cc di cc di cc di cc di cc di	22 23 24 24 24 24 25 25 25 26 26 26 26 26 26 26 26 26 26 26 26 26	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih oc7	3 4 5 5 6 6		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806 1.401832		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6 dih6 oc7		1.54452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804 1.395207	cc cc cc di cc di cc cc di cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 24 24 24 25 25 25 25 26 26 26 26 26 27	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002 0.006625	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih oc7 occ	3 4 5 5 6 6 7		1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806 1.401832 110.488		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6 dih6 oc7 occ7		1.54452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804 1.395207 106.620	cc cc cc di cc cc di cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 24 24 24 25 25 25 25 25 26 26 27 27 27 27	-0.0010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002 0.006625 3.868	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih oc7 occ dih	3 4 5 5 6 6 7 7	_	1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806 1.401832 110.488 127.841		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6 dih6 oc7 occ7 dih7		1.514452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804 1.395207 106.620 -126.425	di cc cc di cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 24 24 24 25 25 25 25 26 25 26 26 27 26 7 26 7 26	-0.010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002 0.006625 3.868 -1.416	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih oc7 occ dih oc8	3 4 4 5 5 6 6 7 7	_	1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806 1.401832 110.488 127.841 1.212674		cc3 cc3 cc4 cc4 dih4 cc5 ccc5 dih5 cc6 ccc6 dih6 oc7 occ7 dih7 oc8		1.514452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804 1.395207 106.620 -126.425 1.210367	di cc cc di cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 23 24 24 24 25 25 25 25 26 25 26 26 27 27 27 28	-0.010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002 0.006625 3.868 -1.416 0.002307	
ccc cc4 ccc dih cc5 ccc dih cc6 ccc dih oc7 occ dih oc8 occ	3 4 5 5 6 6 7 7 8	_	1.514532 103.425 1.337265 112.237 -6.464 1.481690 109.877 1.624 1.539062 110.853 115.806 1.401832 110.488 127.841 1.212674 123.906		cc3 cc3 cc4 cc4 dih4 cc5 cc5 dih5 cc6 cc6 dih6 oc7 occ7 dih7 oc8 occ8		1.514452 102.091 1.338301 113.698 -6.645 1.473990 109.740 1.751 1.533621 109.773 112.804 1.395207 106.620 -126.425 1.210367 125.262	di cc cc di cc cc di cc cc di cc cc di cc cc cc cc cc cc cc cc cc cc cc cc cc	22 33 44 44 44 45 52 46 46 52 52 66 52 66 52 66 52 67 52 67 52 68 52 52 52 52 52 52 52 52 52 52	-0.010233 0.000080 1.334 -0.001036 -1.461 0.181 0.007700 0.137 -0.127 0.005441 1.08 3.002 0.006625 3.868 -1.416 0.002307 -1.356	

cc9	1.386222	cc9	1.351774	cc9	0.034448
ccc9	127.237	ccc9	128.133	ccc9	-0.896
dih9	67.239	dih9	72.858	dih9	-5.619
cc10	1.555429	cc10	1.543617	cc10	0.011812
ccc10	125.638	ccc10	128.133	ccc10	-2.495
dih10	-176.166	dih10	180.000	dih10	3.834
cc11	1.512739	cc11	1.514452	cc11	-0.001713
ccc11	102.446	ccc11	102.091	ccc11	0.355
dih11	170.368	dih11	169.581	dih11	0.787
cc12	1.352453	cc12	1.338301	cc12	0.014152
ccc12	110.787	ccc12	113.698	ccc12	-2.911
dih12	7.781	dih12	6.645	dih12	1.136
cc13	1.436864	cc13	1.473990	cc13	-0.037126
ccc13	109.491	ccc13	109.740	ccc13	-0.249
dih13	-3.622	dih13	-1.751	dih13	-1.871
cc14	1.536000	cc14	1.533621	cc14	0.002379
ccc14	111.525	ccc14	112.428	ccc14	-0.903
dih14	107.614	dih14	108.921	dih14	-1.307
oc15	1.395025	oc15	1.395207	oc15	-0.000182
occ15	113.770	occ15	113.920	occ15	-0.15
dih15	-125.342	dih15	-123.160	dih15	-2.182
oc16	1.341229	oc16	1.210367	oc16	0.130862
occ16	129.629	occ16	127.622	occ16	2.007
dih16	-174.954	dih16	-171.226	dih16	-3.728

Γable S2. z-matrices for the he	y atoms of the S_0 -FC and the ³ P	$P(p_0\pi^*)$ fully optimized structures.
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Model-1

		FC				Sy	$m^{-1}n\pi^{*}(S_{1})$			Sy	$m^{-3}n\pi^{*}(T_{1})$	
С	-0.57749	0.35104	0.00996		С	-0.60247	0.34874	-0.03009	С	-0.598308	0.346792	-0.029199
C	-0.76368	1.88188	-0.05797		C	-0.77576	1.88466	-0.12614	С	-0.774467	1.882798	-0.123897
C	-1.95893	-0.24793	0.06105		С	-1.92964	-0.20275	-0.01066	С	-1.931566	-0.20788	-0.009197
C	-2.25884	2.01088	-0.26149		C	-2.26824	2.03665	-0.32332	С	-2.267087	2.032541	-0.32167
C	-2.91593	0.84832	-0.17354		C	-2.91015	0.86077	-0.21530	С	-2.909762	0.857621	-0.215392
C	-0.35542	2.57937	1.24542		C	-0.36273	2.59267	1.17132	С	-0.360826	2.591087	1.173035
Н	-2.69387	2.97648	-0.43631		Н	-2.71035	2.99918	-0.48993	С	0.598308	-0.346792	0.029199
Н	-3.97260	0.68266	-0.24928		Н	-3.96535	0.67955	-0.26926	С	0.774467	-1.882798	0.123897
Н	-0.86947	2.14780	2.09766		Н	-0.90721	2.19033	2.01818	С	1.931566	0.20788	0.009197
Н	0.71096	2.50283	1.41206		Н	0.69623	2.48635	1.36673	С	2.267087	-2.032541	0.32167
Н	-0.61314	3.63134	1.18243		Н	-0.58590	3.65103	1.08638	С	2.909762	-0.857621	0.215392
Н	0.78552	2.43976	-1.04842		Н	0.78932	2.49616	-1.09165	С	0.360826	-2.591087	-1.173035
0	-2.25626	-1.40315	0.26611		0	-2.27131	-1.41782	0.15643	Н	-2.709594	2.995159	-0.48727
0	-0.15747	2.47691	-1.16479		0	-0.14642	2.45105	-1.23963	Н	-3.964941	0.677262	-0.271558
C	0.57749	-0.35104	-0.00996		C	0.60247	-0.34874	0.03009	Н	-0.904244	2.188486	2.020445
C	0.76368	-1.88188	0.05797		C	0.77576	-1.88466	0.12614	Н	0.698398	2.485371	1.36748
C	1.95893	0.24793	-0.06105		C	1.92964	0.20275	0.01066	Н	-0.584566	3.649345	1.088181
C	2.25884	-2.01088	0.26149		C	2.26824	-2.03665	0.32332	Н	0.789687	2.49279	-1.090737
C	2.91593	-0.84832	0.17354		C	2.91015	-0.86077	0.21530	Н	2.709594	-2.995159	0.48727
C	0.35542	-2.57937	-1.24542		C	0.36273	-2.59267	-1.17132	Н	3.964941	-0.677262	0.271558
Н	2.69387	-2.97648	0.43631		Н	2.71035	-2.99918	0.48993	Н	0.904244	-2.188486	-2.020445
Н	3.97260	-0.68266	0.24928		Н	3.96535	-0.67955	0.26926	Н	-0.698398	-2.485371	-1.36748
Н	0.86947	-2.14780	-2.09766		Н	0.90721	-2.19033	-2.01818	Н	0.584566	-3.649345	-1.088181
Н	-0.71096	-2.50283	-1.41206		Н	-0.69623	-2.48635	-1.36673	Н	-0.789687	-2.49279	1.090737
Н	0.61314	-3.63134	-1.18243		Н	0.58590	-3.65103	-1.08638	0	-2.271981	-1.418734	0.158624
Н	-0.78552	-2.43976	1.04842		Н	-0.78932	-2.49616	1.09165	0	-0.146445	2.449916	-1.237591
0	2.25626	1.40315	-0.26611		0	2.27131	1.41782	-0.15643	0	2.271981	1.418734	-0.158624
0	0.15747	-2.47691	1.16479		0	0.14642	-2.45105	1.23963	0	0.146445	-2.449916	1.237591

	Mi	$n^{-3}\pi\pi^{*}(T_{1})$		1		Mi	$n^{-1}n\pi^{*}(S_{1})$		1		Mi	$n^{-3}n\pi^{*}(T_{1})$	
С	-0.71770	-0.25240	0.00250	1	С	-2.12089	0.93031	-0.62302	1	С	-2.11858	0.93639	-0.62357
C	-1.96980	0.62570	0.03660		C	-2.30054	2.45180	-0.76084		С	-2.29948	2.45775	-0.75639
C	-1.13140	-1.63700	-0.03010		С	-3.47378	0.33459	-0.57246		С	-3.47545	0.33606	-0.57628
C	-3.06520	-0.40810	0.21350		С	-3.79181	2.57705	-0.99716		С	-3.79053	2.57955	-0.99545
C	-2.60450	-1.66210	0.13740		С	-4.44163	1.41624	-0.86084		С	-4.44093	1.41764	-0.86512
C	-2.19233	1.39017	-1.27461		С	-1.21642	-1.93686	-1.92558		С	-1.22431	-1.93349	-1.92705
Н	-4.08453	-0.10335	0.35098		С	-1.92032	3.22206	0.50994		С	-1.92326	3.22641	0.51681
Н	-3.16270	-2.57589	0.19163		С	-0.74526	-1.32372	-0.59927		С	-0.74523	-1.31859	-0.60389
Н	-3.14663	1.90381	-1.22603		С	0.75440	-1.49666	-0.47903		С	0.75556	-1.48651	-0.49330
Н	-1.41928	2.12955	-1.43591		С	1.38715	-0.30167	-0.53779		С	1.38820	-0.29291	-0.53902
Н	-2.20731	0.71365	-2.12246		С	0.38708	0.73047	-0.62022		С	0.39203	0.74260	-0.62545
Н	-1.37840	2.18630	0.99270		С	-0.91441	0.22459	-0.60093		С	-0.91443	0.22771	-0.61039
0	-0.42084	-2.62555	-0.18530		Н	1.20685	-2.46458	-0.39948		Н	1.20831	-2.45420	-0.40943
0	-2.00347	1.48575	1.13825		Н	2.44332	-0.11845	-0.51198		Н	2.44401	-0.10953	-0.50474
C	0.71770	0.25240	-0.00250		Н	-4.22562	3.53469	-1.21370		Н	-4.22522	3.53662	-1.21276
C	1.96980	-0.62570	-0.03660		Н	-5.49656	1.23955	-0.93620		Н	-5.49563	1.24174	-0.94499
C	1.13140	1.63700	0.03010		Н	-0.99838	-2.99943	-1.92112		Н	-1.00035	-2.99479	-1.92337
C	3.06520	0.40810	-0.21350		Н	-2.28216	-1.81380	-2.06379		Н	-2.29167	-1.81686	-2.05632
C	2.60450	1.66210	-0.13740		Н	-0.70461	-1.48062	-2.76598		Н	-0.72113	-1.47569	-2.77187
C	2.19233	-1.39017	1.27461		Н	-2.46477	2.84093	1.36615		Н	-2.46085	2.83793	1.37454
Н	4.08453	0.10335	-0.35098		Н	-0.86180	3.14703	0.72724		Н	-0.86318	3.16260	0.73029
Н	3.16270	2.57589	-0.19163		Н	-2.16611	4.27153	0.38316		Н	-2.17787	4.27375	0.39296
Н	3.14663	-1.90381	1.22603		Н	-2.28377	-1.87513	0.40667		Н	-2.27530	-1.87134	0.41233
Н	1.41928	-2.12955	1.43591		Н	-0.75673	3.19075	-1.70715		Н	-0.72943	3.05539	-1.74112
Н	2.20731	-0.71365	2.12246		0	0.75351	2.04125	-0.66860		0	0.73940	2.04911	-0.62252
Н	1.37840	-2.18630	-0.99270		0	-3.77921	-0.81431	-0.32262		0	-3.77504	-0.81342	-0.32564
0	0.42084	2.62555	0.18530		0	-1.34001	-1.95053	0.49473		0	-1.33060	-1.94716	0.49388
0	2.00347	-1.48575	-1.13825		0	-1.66384	2.98967	-1.89129		0	-1.66535	2.99998	-1.88331

Γ		3	$^{3}P(p_{0}\pi^{*})$		1		1	$I^*(n'\pi^*)$:	$J^*(n'\pi^*)$	
Г	С	-2.18615	0.94423	-0.67205	1	С	-2.17761	0.95351	-0.70514	С	-2.17167	0.95030	-0.68553
	С	-2.32842	2.49029	-0.76595		С	-2.32839	2.49798	-0.76929	С	-2.32480	2.49468	-0.76351
	С	-3.51041	0.43948	-0.62751		С	-3.49868	0.43874	-0.65247	С	-3.49822	0.43426	-0.63624
	С	-3.81363	2.66790	-0.99176		С	-3.81734	2.66893	-0.97991	С	-3.81048	2.66234	-0.99412
	С	-4.46375	1.48951	-0.85802		С	-4.46089	1.48386	-0.85243	С	-4.45382	1.47604	-0.86792
	С	-1.26061	-1.96640	-1.94590		С	-1.24431	-1.97267	-1.97144	С	-1.26294	-1.96640	-1.95563
	С	-1.93566	3.17349	0.55249		С	-1.92951	3.15953	0.55840	С	-1.93859	3.16686	0.56216
	С	-0.80832	-1.27975	-0.64488		С	-0.82734	-1.27109	-0.67563	С	-0.82195	-1.26826	-0.66714
	С	0.68112	-1.45414	-0.43286		С	0.65701	-1.45342	-0.41280	С	0.66860	-1.45337	-0.43486
	С	1.33695	-0.28923	-0.46687		С	1.32240	-0.29286	-0.44962	С	1.33477	-0.29392	-0.46889
	С	0.37838	0.82295	-0.66587		С	0.38251	0.82665	-0.68801	С	0.39159	0.82921	-0.67894
	С	-0.99067	0.24271	-0.65460		С	-0.98724	0.24923	-0.71092	С	-0.97966	0.25434	-0.68831
	Н	1.10754	-2.43167	-0.30859		Н	1.07604	-2.43144	-0.27294	Н	1.09084	-2.43279	-0.31424
	Н	2.39332	-0.12587	-0.38273		Н	2.37999	-0.14565	-0.35130	Н	2.39351	-0.14745	-0.38361
	Н	-4.24226	3.63531	-1.16236		Н	-4.25400	3.63520	-1.13586	Н	-4.24759	3.62730	-1.15646
	Н	-5.52087	1.31630	-0.90889		Н	-5.51770	1.30673	-0.89512	Н	-5.50987	1.29787	-0.92354
	Н	-1.04861	-3.02925	-1.89872		Н	-1.02002	-3.03164	-1.89815	Н	-1.04305	-3.02714	-1.88891
	Н	-2.31850	-1.82579	-2.11519		Н	-2.30424	-1.85669	-2.14897	Н	-2.32443	-1.84595	-2.11943
	Н	-0.71268	-1.54102	-2.77709		Н	-0.70333	-1.55828	-2.81419	Н	-0.73215	-1.55563	-2.80696
	Н	-2.50761	2.77022	1.38117		Н	-2.49058	2.73709	1.38497	Н	-2.50773	2.75123	1.38662
	Н	-0.88233	3.04982	0.76669		Н	-0.87333	3.03938	0.76071	Н	-0.88441	3.04726	0.77548
	Н	-2.14139	4.23588	0.47549		Н	-2.14315	4.22162	0.50278	Н	-2.15103	4.22860	0.49592
	Н	-3.29790	-1.33247	0.02263		Н	-3.39386	-1.30431	0.14168	Н	-3.39846	-1.33988	0.10084
	Н	-0.72178	3.01881	-1.67558		Н	-0.72846	3.03861	-1.68410	Н	-0.71613	3.03516	-1.66446
	0	0.70710	1.98026	-0.81800		0	0.71942	1.98048	-0.84492	0	0.72811	1.98497	-0.82045
	0	-3.94086	-0.81897	-0.45450		0	-3.90379	-0.83873	-0.51217	0	-3.92072	-0.84048	-0.51327
	0	-1.52711	-1.91439	0.37772		0	-1.48007	-1.84271	0.42185	0	-1.47051	-1.81799	0.44923
	0	-1.65501	3.05205	-1.85086		0	-1.66367	3.08223	-1.84759	0	-1.64937	3.06912	-1.84040

		${}^{1}P(n'\pi^{*})$		1			$^{3}P(n'\pi^{*})$		1			¹ P(Epox)	
С	-2.15634	0.95311	-0.73652	1	С	-2.15372	0.94881	-0.72963	1	С	-2.184373	0.991333	-0.9409
C	-2.32596	2.49676	-0.73990		С	-2.32359	2.49354	-0.73396		C	-2.327589	2.526685	-0.78238
C	-3.46253	0.41769	-0.67889		С	-3.46429	0.41566	-0.68115		С	-3.448177	0.499179	-0.895901
C	-3.82825	2.66010	-0.83635		С	-3.82404	2.65908	-0.84014		С	-3.801383	2.738611	-1.061318
C	-4.44868	1.45584	-0.75757		С	-4.44643	1.45712	-0.76688		С	-4.44754	1.566716	-1.063574
C	-1.14858	-2.04026	-1.90068		С	-1.16255	-2.05392	-1.87069		С	-1.434515	-2.245199	-1.691373
С	-1.83692	3.11977	0.57536		С	-1.84117	3.11707	0.58364		С	-2.053831	2.96937	0.667035
С	-0.78057	-1.26336	-0.63071		С	-0.76598	-1.26052	-0.61872		С	-0.683813	-1.243704	-0.847901
С	0.71069	-1.39397	-0.36064		С	0.73185	-1.38884	-0.38709		С	0.815925	-1.428784	-0.806696
С	1.35803	-0.22965	-0.49036		С	1.37190	-0.22103	-0.51493		С	1.436956	-0.261351	-0.59374
С	0.39626	0.85212	-0.80019		С	0.39945	0.85972	-0.79605		С	0.438035	0.830178	-0.555652
С	-0.96193	0.25421	-0.75500		С	-0.95754	0.25645	-0.74147		С	-0.948849	0.200481	-0.659192
Н	1.14791	-2.35174	-0.15225		Н	1.17369	-2.34710	-0.19076		Н	1.278502	-2.394098	-0.888182
Н	2.41392	-0.05852	-0.41385		Н	2.42763	-0.04336	-0.45325		Н	2.48679	-0.079519	-0.475656
Н	-4.28848	3.62429	-0.91838		Н	-4.28193	3.62457	-0.92058		Н	-4.213746	3.723407	-1.16083
Н	-5.50926	1.28166	-0.76662		Н	-5.50740	1.28490	-0.78348		Н	-5.498227	1.379532	-1.165113
н	-0.88746	-3.08521	-1.77073		Н	-0.88548	-3.09466	-1.74143		Н	-1.405317	-3.216571	-1.205333
н	-2.20684	-1.97222	-2.10106		Н	-2.22560	-1.99713	-2.04492		Н	-2.460245	-1.976152	-1.873841
Н	-0.60325	-1.64809	-2.75203		Н	-0.64189	-1.65899	-2.73580		Н	-0.930382	-2.33875	-2.647288
Н	-2.32659	2.66002	1.42716		Н	-2.33744	2.65932	1.43268		Н	-2.68487	2.428487	1.362461
н	-0.76710	3.01025	0.69276		Н	-0.77239	3.00516	0.70809		Н	-1.021099	2.815566	0.948276
Н	-2.06745	4.17983	0.57277		Н	-2.06943	4.17767	0.57841		Н	-2.2688	4.029042	0.75612
Н	-4.63609	-1.04959	-0.37395		Н	-4.67607	-1.03293	-0.46675		Н	-3.265608	-1.167395	-0.041691
Н	-0.80621	3.04237	-1.77705		Н	-0.79912	3.04756	-1.76044		Н	-0.675856	3.273758	-1.42542
0	0.70835	1.99605	-1.05792		0	0.70723	2.00726	-1.04296		0	0.703512	2.006302	-0.548806
0	-3.73745	-0.90035	-0.63564		0	-3.75476	-0.89883	-0.64339		0	-3.881954	-0.7515	-0.634531
0	-1.40814	-1.81652	0.48056		0	-1.38704	-1.81901	0.49571		0	-1.146014	-0.853751	0.413348
0	-1.75121	3.12568	-1.84492		0	-1.74404	3.12272	-1.83667		0	-1.587666	3.298403	-1.684509
	1	¹ <i>I</i> *(<i>n'</i> π*)				3	I*(n'π*)				¹ <i>P</i>	(EpoxRot)	
C	-2.17761	1 Ι*(n'π*) 0.95351	-0.70514		С	-2.17167	Ι*(n'π*) 0.95030	-0.68553		С	¹ P(-2.35949	(EpoxRot) 0.63598	-0.330648
C C	-2.17761 -2.32839	1*(n'π*) 0.95351 2.49798	-0.70514 -0.76929		C C	-2.17167 -2.32480	Π*(n'π*) 0.95030 2.49468	-0.68553 -0.76351		C C	¹ <i>P</i> (-2.35949 -2.48364	(EpoxRot) 0.63598 1.97568	-0.330648 -1.06386
C C C	-2.17761 -2.32839 -3.49868	1^μ(n'π*) 0.95351 2.49798 0.43874	-0.70514 -0.76929 -0.65247		C C C	-2.17167 -2.32480 -3.49822	Π*(n'π*) 0.95030 2.49468 0.43426	-0.68553 -0.76351 -0.63624		C C C	-2.35949 -2.48364 -3.548985	(EpoxRot) 0.63598 1.97568 0.336369	-0.330648 -1.06386 0.220752
C C C C	-2.17761 -2.32839 -3.49868 -3.81734	<i>T</i>*(<i>n'</i>π*) 0.95351 2.49798 0.43874 2.66893	-0.70514 -0.76929 -0.65247 -0.97991		C C C C	-2.17167 -2.32480 -3.49822 -3.81048	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.42604	-0.68553 -0.76351 -0.63624 -0.99412		C C C C	-2.35949 -2.48364 -3.548985 -3.956987	(EpoxRot) 0.63598 1.97568 0.336369 2.294701	-0.330648 -1.06386 0.220752 -0.893236
C C C C C	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089	1 *(<i>n</i> ′π*) 0.95351 2.49798 0.43874 2.66893 1.48386	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243		C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792		C C C C C	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927	-0.330648 -1.06386 0.220752 -0.893236 -0.130708
C C C C C C C C C	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 2.16522	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144		C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 2.4620	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563		C C C C C C C	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114
	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 0.82324	H*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 1.25730	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840		C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -9.93105	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 1.26826	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216		C C C C C C C C C C C	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 0.42325	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 0.042564	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407
	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 1.45322	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563		C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.46826	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714		C C C C C C C C C C C C C C C C C C C	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 0.972467	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.22045
	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.23240	If*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 0.20366	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 0.44062		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.23477	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 0.20202	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 0.46880		С С С С С С С С С С С С С С С С С С С	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24820	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 0.332925	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317
	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.22551	1 *(n'\pi *) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.9265	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.69901		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.20150	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 0.478904		с с с с с с с с с с с с с с с с с с с	12,35949 -2,48364 -3,548985 -3,956987 -4,552123 -0,859473 -1,616781 -0,432135 1,033882 1,24829 0,026623	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252770	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.706692
	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724	1 *(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894		C C C C C C C C C C C C C C C C C C C	-2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 0.252779 0.42915	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292
ССССССССС	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27994		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43380	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.68831 -0.31424		C C C C C C C C C C C C C C C C C C C	12,35949 -2,48364 -3,548985 -3,956987 -4,552123 -0,859473 -1,616781 -0,432135 1,033882 1,24829 -0,026663 -1,109927 1,769633	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411
СССССССНН	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14555	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361		C C C C C C C C C C C C C C C C C C C	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172772	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.24631	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.82086
СССССССС ССССССС Н Н Н	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14555 3.63520	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.6730	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646		C C C C C C C C C C C C C C C C C C C	127 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402776	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.160041	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.32551
C C C C C C C C C C C C C C C C C C C	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5 50987	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354		C C C C C C C C C C C C C C C C C C C	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5 580098	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892		C C C C C C C C C C C C H H H H H H	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101
ССССССССННННН	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.85669	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897		C C C C C C C C C C C C C C C C C C C	3 -2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443	I*(n'\pi *) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944		C C C C C C C C C C C C H H H H H H H H	19/ -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -0.221561	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.85669 -1.55828	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697		С С С С С С С С С С С С С С С С С С С	19/ -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.32225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -0.947489 -0.424684	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058	I*(n'\pi *) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662		C C C C C C C C C C C C C H H H H H H H	12,35949 -2,48364 -3,548985 -3,956987 -4,552123 -0,859473 -1,616781 -0,432135 1,033882 1,24829 -0,026663 -1,109927 1,769633 2,172272 -4,402726 -5,580098 -0,628999 -1,921561 -0,329643 -1,809406	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.32225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677
С С С С С С С С С С С С С С С И Н Н Н Н	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333	1 *(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.52443 -0.73215 -2.50773 -0.88441	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 2.75123 3.04726	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548		C C C C C C C C C C C C C H H H H H H H	120 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.32225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.9424684 3.181646 2.851692	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466
С С С С С С С С С С С С С С И Н Н Н Н Н	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333 -2.14315	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.85669 2.73709 3.03938 4.22162	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071 0.50278		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 2.75123 3.04726 4.22860	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592		С С С С С С С С С С С С С С С С С С С	120 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428
С С С С С С С С С С С С С С С И Н Н Н Н	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333 -2.14315 -3.39386	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938 4.22162 -1.30431	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071 0.50278 0.14168		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103 -3.39846	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.5434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123 3.04726 4.22860 -1.33988	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592 0.10084		С С С С С С С С С С С С С С С С С С С	127 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538 -4.747228	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726 -0.802601	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428 1.156067
С С С С С С С С С С С С С С С С И Н Н Н Н	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333 -2.14315 -3.39386 -0.72846	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938 4.22162 -1.30431 3.03861	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 -2.81419 1.38497 0.76071 0.50278 0.14168 -1.68410		С С С С С С С С С С С С С С С С С С С	3 -2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103 -3.39846 -0.71613	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123 3.04726 4.22860 -1.33988 3.03516	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592 0.10084 -1.66446		С С С С С С С С С С С С И Н Н Н Н Н Н Н	127 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538 -4.747228 -1.28343	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726 -0.802601 1.863664	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428 1.1550667 -2.588596
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.70333 -2.14315 -3.39386 -0.72846 0.71942	I*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938 4.22162 -1.30431 3.03861 1.98048	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071 0.50278 0.14168 -1.68410 -0.84492		С С С С С С С С С С С С С С С С С С С	3 -2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103 -3.39846 -0.71613 0.72811	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123 3.04726 4.22860 -1.3988 3.03516 1.98497	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.67894 -0.67894 -0.31424 -0.33861 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592 0.10084 -1.66446 -0.82045		C C C C C C C C C C C C H H H H H H H H	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538 -4.747228 -1.28343 -1.12843 -0.17000	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726 -0.802601 1.863664 0.948233	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428 1.156067 -2.588596 1.772759
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333 -2.49058 -0.87333 -2.14315 -3.39386 -0.72846 0.71942 -3.90379	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938 4.22162 -1.30431 3.03861 1.98048 -0.83873	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071 0.50278 0.14168 -1.68410 -0.84492 -0.51217		С С С С С С С С С С С С С С С С С С С	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103 -3.39846 -0.71613 0.72811 -3.92072	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123 3.04726 4.22860 -1.3988 3.03516 1.98497 -0.84048	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592 0.10084 -1.66446 -0.82045 -0.51327		C C C C C C C C C C C C H H H H H H H H	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538 -4.747228 -1.28343 -0.17000 -3.81604	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726 -0.802601 1.8633664 0.948233 -0.722541	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428 1.156067 -2.588596 1.772759 1.005545
С С С С С С С С С С С С С С С С С С С	-2.17761 -2.32839 -3.49868 -3.81734 -4.46089 -1.24431 -1.92951 -0.82734 0.65701 1.32240 0.38251 -0.98724 1.07604 2.37999 -4.25400 -5.51770 -1.02002 -2.30424 -0.70333 -2.49058 -0.87333 -2.14315 -3.39386 -0.72846 0.71942 -3.90379 -1.48007	μ*(n'π*) 0.95351 2.49798 0.43874 2.66893 1.48386 -1.97267 3.15953 -1.27109 -1.45342 -0.29286 0.82665 0.24923 -2.43144 -0.14565 3.63520 1.30673 -3.03164 -1.55828 2.73709 3.03938 4.22162 -1.30431 3.03861 1.98048 -0.83873 -1.84271	-0.70514 -0.76929 -0.65247 -0.97991 -0.85243 -1.97144 0.55840 -0.67563 -0.41280 -0.44962 -0.68801 -0.71092 -0.27294 -0.35130 -1.13586 -0.89512 -1.89815 -2.14897 -2.81419 1.38497 0.76071 0.50278 0.14168 -1.68410 -0.84492 -0.51217 0.42185		C C C C C C C C C C C C C C C C C C C	-2.17167 -2.32480 -3.49822 -3.81048 -4.45382 -1.26294 -1.93859 -0.82195 0.66860 1.33477 0.39159 -0.97966 1.09084 2.39351 -4.24759 -5.50987 -1.04305 -2.32443 -0.73215 -2.50773 -0.88441 -2.15103 -3.39846 -0.71613 0.72811 -3.92072 -1.47051	I*(n'π*) 0.95030 2.49468 0.43426 2.66234 1.47604 -1.96640 3.16686 -1.26826 -1.45337 -0.29392 0.82921 0.25434 -2.43280 -0.14745 3.62730 1.29787 -3.02714 -1.84595 -1.55563 2.75123 3.04726 4.22860 -1.33988 3.03516 1.98497 -0.84048 -1.81799	-0.68553 -0.76351 -0.63624 -0.99412 -0.86792 -1.95563 0.56216 -0.66714 -0.43486 -0.46889 -0.67894 -0.68831 -0.31424 -0.38361 -1.15646 -0.92354 -1.88892 -2.11944 -2.80697 1.38662 0.77548 0.49592 0.10084 -1.66446 -0.82045 -0.51327 0.44923		С С С С С С С С С С С С С С С С С С О С С С С О С С С О С С О С С О С	194 -2.35949 -2.48364 -3.548985 -3.956987 -4.552123 -0.859473 -1.616781 -0.432135 1.033882 1.24829 -0.026663 -1.109927 1.769633 2.172272 -4.402726 -5.580098 -0.628999 -1.921561 -0.329643 -1.809406 -0.560212 -1.81538 -4.747228 -1.28343 -0.17000 -3.81604 -1.20329	(EpoxRot) 0.63598 1.97568 0.336369 2.294701 1.366927 -1.114821 3.07655 -0.942964 -0.973467 -0.332225 0.252779 -0.142915 -1.501638 -0.246031 3.169041 1.34563 -2.124064 -0.947489 -0.424684 3.181646 2.851692 4.020726 -0.802601 1.863664 0.948233 -0.722541 -1.604838	-0.330648 -1.06386 0.220752 -0.893236 -0.130708 -2.654114 -0.446407 -1.223049 -0.857445 0.304317 0.799692 -0.19292 -1.434411 0.842086 -1.325651 0.181456 -2.981101 -2.760379 -3.303056 0.613677 -0.569466 -0.942428 1.156067 -2.588596 1.772759 1.005545 -0.255518

Madal 3

		FC]		М	$\ln^{-1}n\pi^{*}(S_{1})$]		М	$in^{-3}n\pi^{*}(T_{1})$	
C	-5.29861	0.96873	0.10950]	С	-5.27946	1.00927	0.21146		С	-5.27092	1.003366	0.216967
C	5.29861	-0.96873	-0.10950		C	-4.06381	1.62237	-0.01852		C	-4.056531	1.618994	-0.009471
C	-4.07783	1.59946	-0.03530		C	-2.93291	0.82090	-0.09015		C	-2.924199	0.818971	-0.086205
C	4.07783	-1.59946	0.03530		C	-3.00171	-0.54757	0.04773		C	-2.990841	-0.550019	0.043077
C	-2.93112	0.80161	-0.07986		C	-4.21810	-1.16625	0.28948		C	-4.20699	-1.171708	0.281234
C	2.93112	-0.80161	0.07986		C	-5.35086	-0.37548	0.36998		C	-5.340255	-0.382969	0.366664
C	-2.98929	-0.56523	0.00186		C	-1.64282	-1.20501	-0.12446		C	-1.632371	-1.207463	-0.129063
C	2.98929	0.56523	-0.00186		C	-1.52382	1.23238	-0.27161		C	-1.517734	1.234616	-0.268412
C	-4.21702	-1.20765	0.15959		C	-0.69706	0.01034	-0.16082		С	-0.683712	0.008898	-0.164162
C	4.21702	1.20765	-0.15959		C	-1.61240	-2.00114	-1.43729		С	-1.602189	-2.00569	-1.440374
C	-5.36313	-0.43170	0.21156		C	5.34023	-0.95933	-0.00221		C	5.324698	-0.975556	-0.003263
C	5.36313	0.43170	-0.21156		C	4.10856	-1.59635	0.02220		С	4.08184	-1.602668	0.020805
C	-1.62362	-1.21934	-0.10996		C	2.96289	-0.79481	0.00917		C	2.945885	-0.796128	0.0103
C	1.62362	1.21934	0.10996		C	3.03928	0.57589	-0.01247		C	3.031202	0.5852	-0.009778
C	-1.52978	1.23693	-0.18379		C	4.27589	1.21094	-0.04888		C	4.264065	1.210835	-0.047308
C	1.52978	-1.23693	0.18379		C	5.41741	0.43824	-0.04396		C	5.416976	0.420046	-0.043215
C	-0.67024	0.00151	-0.06780		C	1.65984	1.20778	0.02356		С	1.652308	1.219013	0.023489
C	0.67024	-0.00151	0.06780		C	1.54705	-1.15367	-0.02431		С	1.542148	-1.143992	-0.023573
C	-1.50847	-1.97487	-1.44149		C	0.71572	-0.02416	-0.08156		С	0.70939	-0.017923	-0.082217
C	1.50847	1.97487	1.44149		C	1.46354	1.93627	1.36151		С	1.452257	1.947448	1.360484
Н	-6.20395	1.54642	0.15278		Н	-6.17639	1.59788	0.27783		Н	-6.168698	1.590199	0.287268
H	6.20395	-1.54642	-0.15278		Н	-3.98424	2.68788	-0.13064		Н	-3.97798	2.685215	-0.115337
H	-3.99900	2.66847	-0.10398		Н	-4.28033	-2.23018	0.42385		Н	-4.267702	-2.236453	0.409087
H	3.99900	-2.66847	0.10398		Н	-6.30469	-0.83388	0.56097		Н	-6.29352	-0.84377	0.55472
H	-4.26890	-2.27621	0.25223		Н	-0.63978	-2.44424	-1.61505		Н	-0.63107	-2.452787	-1.615994
H	4.26890	2.27621	-0.25223		Н	-2.34794	-2.79720	-1.39614		Н	-2.339675	-2.799657	-1.398808
H	-6.32004	-0.90601	0.33618		Н	-1.84734	-1.36032	-2.27883		Н	-1.833239	-1.365293	-2.283592
H	6.32004	0.90601	-0.33618		Н	-0.76194	-2.68355	0.80221		Н	-0.701593	-2.625939	0.841151
H	-0.53157	-2.42815	-1.54741		Н	6.24367	-1.54162	0.00249		Н	6.220588	-1.569459	0.000323
H	0.53157	2.42815	1.54741		Н	4.04236	-2.66876	0.04179		Н	4.005959	-2.674494	0.037187
H	-2.25362	-2.76191	-1.47302		Н	4.33707	2.28257	-0.09331		Н	4.333813	2.281849	-0.091771
H	2.25362	2.76191	1.47302		н	6.38220	0.91171	-0.07626		н	6.384317	0.887465	-0.075222
H	-1.67366	-1.31071	-2.28280		н	0.47356	2.36678	1.43206		н	0.462809	2.378751	1.429695
H	1.67366	1.31071	2.28280		H	2.18633	2.74053	1.43978		Н	2.176531	2.750314	1.43951
H	-0.65729	-2.52647	0.91208		н	1.60693	1.25910	2.19613		н	1.594093	1.270384	2.195503
H	0.65729	2.52647	-0.91208		H	0.70647	2.50454	-1.02027		Н	0.702067	2.513438	-1.024477
0	-1.16583	2.38264	-0.33130		0	-1.15400	2.37186	-0.47667		0	-1.152417	2.374124	-0.473691
0	1.16583	-2.38264	0.33130		0	-1.43583	-2.04255	0.98207		0	-1.435732	-2.04299	0.980243
0	-1.49552	-2.08193	0.97729		0	1.18560	-2.44778	-0.03750		0	1.170308	-2.428926	-0.056769
0	1.49552	2.08193	-0.97729	1	0	1.56083	2.08658	-1.05335		0	1.556116	2.094756	-1.055006

	М	in- $^{3}\pi\pi^{*}(T_{1})$		$\frac{\text{Sym-}^{1}n\pi^{*}(\text{S}_{1})}{\text{Sym-}^{1}n\pi^{*}(\text{S}_{1})}$					Sy	$m^{-3}n\pi^{*}(T_{1})$		
С	-5.346174	0.97747	0.144532	1	С	-5.308837	0.954704	0.167276	С	-5.306657	0.95624	0.169083
C	5.346174	-0.97747	-0.144532		С	5.308837	-0.954704	-0.167276	С	5.306657	-0.95624	-0.169083
C	-4.139763	1.604876	0.00699		С	-4.1031	1.583414	0.025246	С	-4.101487	1.585946	0.02866
C	4.139763	-1.604876	-0.00699		С	4.1031	-1.583414	-0.025246	С	4.101487	-1.585946	-0.02866
C	-2.985442	0.80538	-0.032315		С	-2.947341	0.783656	-0.010786	С	-2.944737	0.787303	-0.008206
C	2.985442	-0.80538	0.032315		С	2.947341	-0.783656	0.010786	С	2.944737	-0.787303	0.008206
C	-3.052261	-0.563683	0.054102		С	-3.017104	-0.586946	0.0815	С	-3.013142	-0.583385	0.08195
C	3.052261	0.563683	-0.054102		С	3.017104	0.586946	-0.0815	С	3.013142	0.583385	-0.08195
C	-4.291851	-1.20413	0.203754		С	-4.254365	-1.223707	0.237076	С	-4.250558	-1.221174	0.235827
C	4.291851	1.20413	-0.203754		С	4.254365	1.223707	-0.237076	С	4.250558	1.221174	-0.235827
C	-5.419368	-0.429094	0.248163		С	-5.384319	-0.449856	0.279308	С	-5.381118	-0.448746	0.278584
C	5.419368	0.429094	-0.248163		С	5.384319	0.449856	-0.279308	С	5.381118	0.448746	-0.278584
C	-1.680718	-1.205606	-0.063681		С	-1.644119	-1.21907	-0.034589	С	-1.641223	-1.217355	-0.034722
C	1.680718	1.205606	0.063681		С	1.644119	1.21907	0.034589	С	1.641223	1.217355	0.034722
C	-1.568562	1.223422	-0.124474		С	-1.5345	1.173949	-0.096482	С	-1.533604	1.181635	-0.096556
C	1.568562	-1.223422	0.124474		С	1.5345	-1.173949	0.096482	С	1.533604	-1.181635	0.096556
C	-0.760468	0.023088	-0.038435		С	-0.704484	0.016437	-0.022481	С	-0.69764	0.015953	-0.022756
C	0.760468	-0.023088	0.038435		С	0.704484	-0.016437	0.022481	С	0.69764	-0.015953	0.022756
C	-1.568729	-1.97208	-1.39062		С	-1.539562	-1.985874	-1.36113	С	-1.537876	-1.986591	-1.35966
C	1.568729	1.97208	1.39062		С	1.539562	1.985874	1.36113	С	1.537876	1.986591	1.35966
Н	-6.253067	1.553608	0.181788		Η	-6.214593	1.532851	0.202854	Н	-6.212822	1.533715	0.205205
Н	6.253067	-1.553608	-0.181788		Н	6.214593	-1.532851	-0.202854	Н	6.212822	-1.533715	-0.205205
Н	-4.064925	2.67422	-0.063982		Н	-4.035861	2.653105	-0.049091	Н	-4.034956	2.655754	-0.044223
Н	4.064925	-2.67422	0.063982		Н	4.035861	-2.653105	0.049091	Н	4.034956	-2.655754	0.044223
Н	-4.350148	-2.272758	0.295675		Н	-4.311194	-2.292036	0.334782	Н	-4.306427	-2.289694	0.331948
Н	4.350148	2.272758	-0.295675		Н	4.311194	2.292036	-0.334782	Н	4.306427	2.289694	-0.331948
Н	-6.381953	-0.893113	0.368208		Н	-6.346498	-0.913108	0.404183	Н	-6.342969	-0.913088	0.401871
Н	6.381953	0.893113	-0.368208		Н	6.346498	0.913108	-0.404183	Н	6.342969	0.913088	-0.401871
Н	-0.585333	-2.406258	-1.512558		Н	-0.553727	-2.409714	-1.501032	Н	-0.552557	-2.411633	-1.499483
Н	0.585333	2.406258	1.512558		Н	0.553727	2.409714	1.501032	Н	0.552557	2.411633	1.499483
Н	-2.297215	-2.775147	-1.398551		Н	-2.260291	-2.796145	-1.364989	Н	-2.259373	-2.796225	-1.361653
Н	2.297215	2.775147	1.398551		Н	2.260291	2.796145	1.364989	Н	2.259373	2.796225	1.361653
Н	-1.767498	-1.320413	-2.234487		Н	-1.751379	-1.331891	-2.199212	Н	-1.749467	-1.333991	-2.198838
Н	1.767498	1.320413	2.234487		Н	1.751379	1.331891	2.199212	Н	1.749467	1.333991	2.198838
Н	-0.67761	-2.519314	0.918754		Н	-0.685124	-2.582845	0.952629	Н	-0.685725	-2.582764	0.953735
Н	0.67761	2.519314	-0.918754		Н	0.685124	2.582845	-0.952629	Н	0.685725	2.582764	-0.953735
0	-1.18063	2.379618	-0.249127		0	-1.180542	2.393494	-0.206828	0	-1.181338	2.395906	-0.208033
0	1.18063	-2.379618	0.249127		0	1.180542	-2.393494	0.206828	0	1.181338	-2.395906	0.208033
0	-1.499045	-2.053016	1.030161		0	-1.474809	-2.068963	1.061838	0	-1.473307	-2.065716	1.063179
0	1.499045	2.053016	-1.030161		0	1.474809	2.068963	-1.061838	0	1.473307	2.065716	-1.063179

Table S3. Cartesian coordinates of the fully optimized structures of Model-1 and Model-2.

Section II: Crystal phase

Geometries optimized at the PBE+D2 in the crystal phase









Figure S10. Geometries of the stationary points located at the PBE+D2 level using PBC.



Figure S11. Spin densities of T_1 at the different stationary points located on T_1