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Electronic Supporting Information

Regioselective [2+2] photocycloaddition reaction of 2-(3,4-dimethoxystyryl)quinoxaline in solution

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Elena O. Guskova, Tseimur M. Aliyev, Nikolai E. Shepel, Yuri V. Fedorov

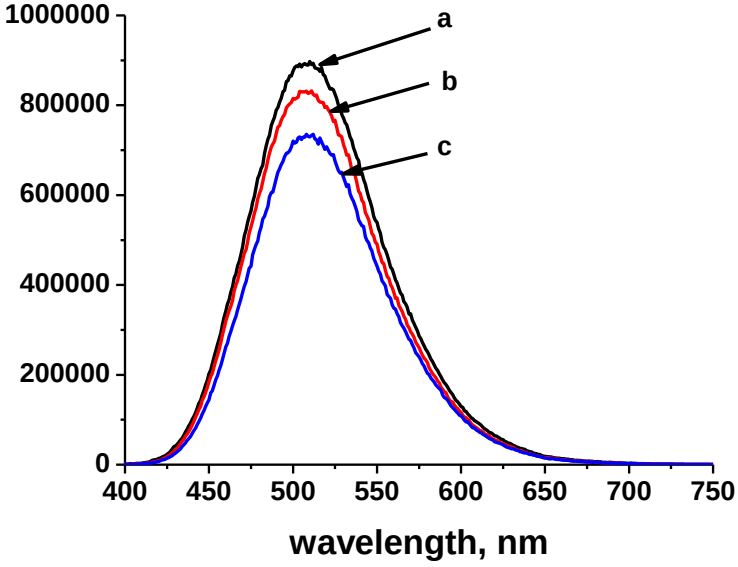


Fig. S1. Fluorescence spectra of **1**, MeCN, 20°C, $C_1 = 1\cdot10^{-5}$ M (a), $C_1 = 1\cdot10^{-3}$ M (b) and $C_1 = 1\cdot10^{-2}$ (c)

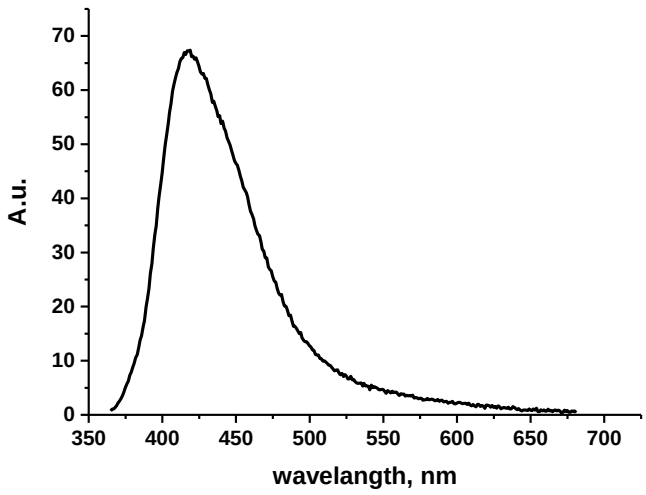
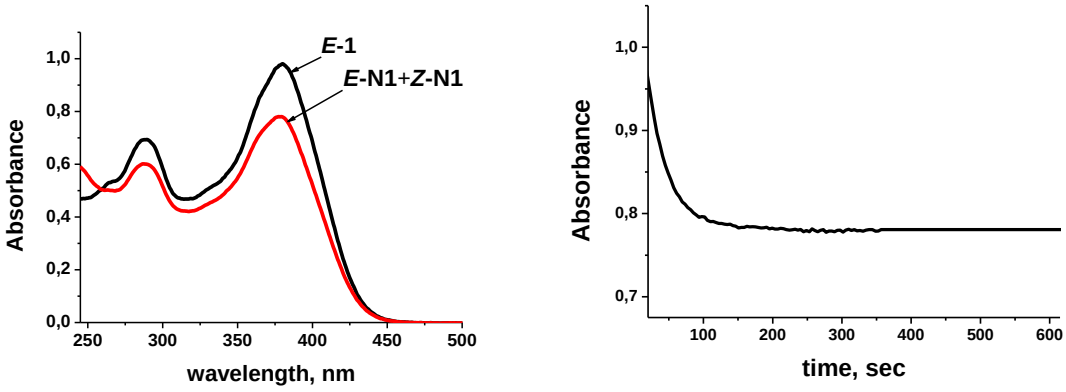
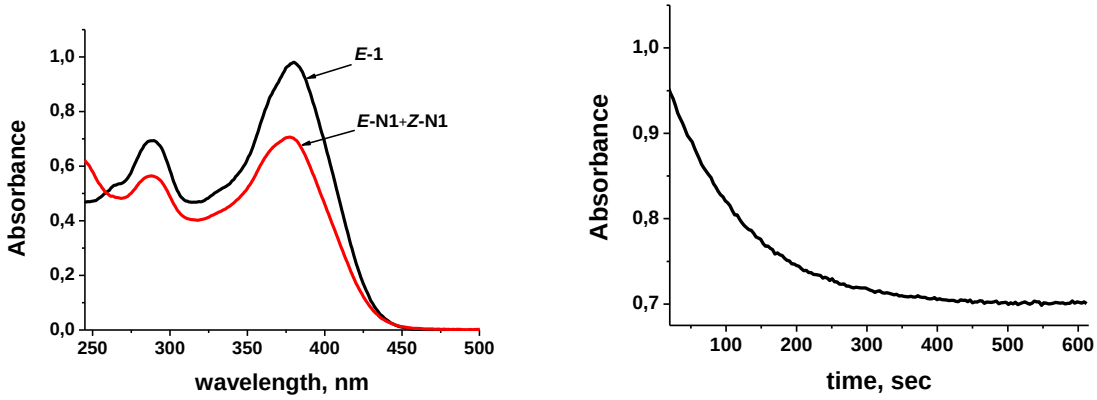


Fig. S2. Fluorescence spectra ***E*-2**, MeCN, 20°C, $C_2 = 4\cdot10^{-5}$

a)



b)



c)

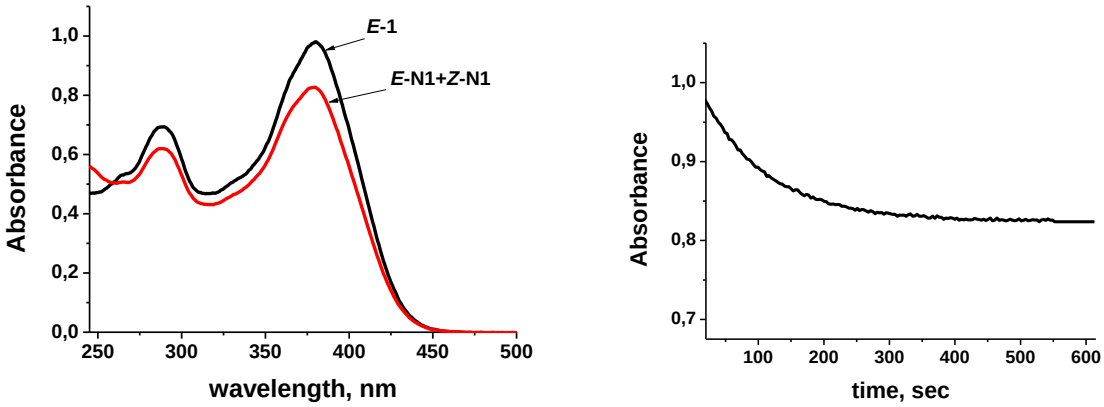
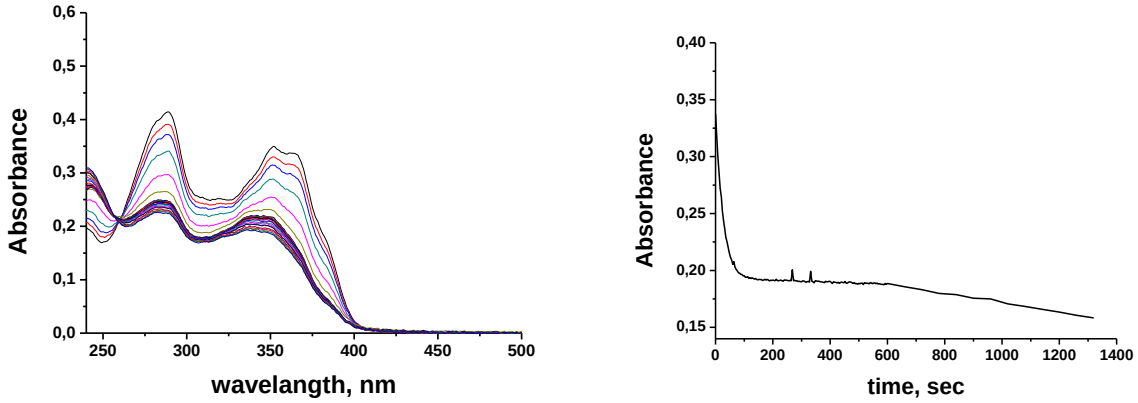


Fig. S3 Spectral changes during photolysis of **1** in acetonitrile with a mercury lamp at different wavelengths: λ = 365nm (a), λ = 405nm (b), λ = 313nm (c). In all cases, $C_{E\text{-}1} = 4{\cdot}10^{-5}$ M.

a)



b)

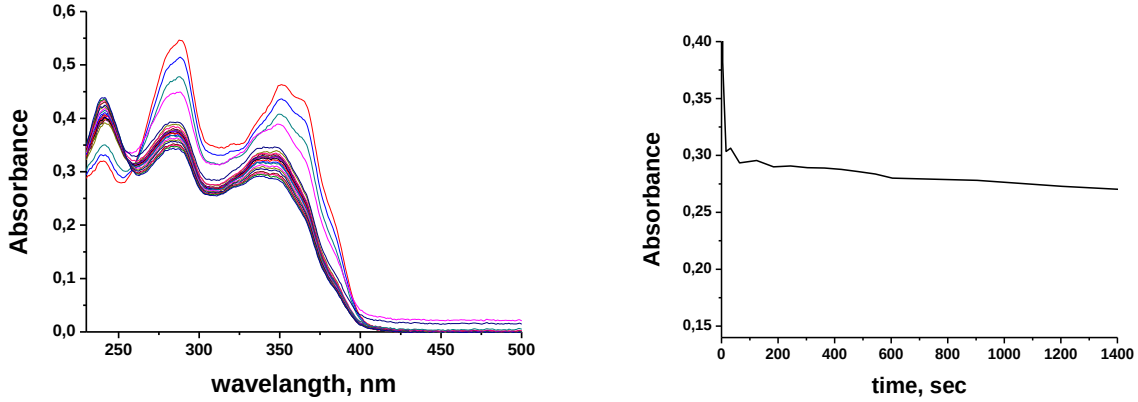


Fig. S4. Spectral changes during photolysis of solution of ***E*-2** in acetonitrile at 365nm, $C_{E\text{-}2}$ = $4{\cdot}10^{-5}$ M (a), $C_{E\text{-}2}$ = $4{\cdot}10^{-4}$ M (b).

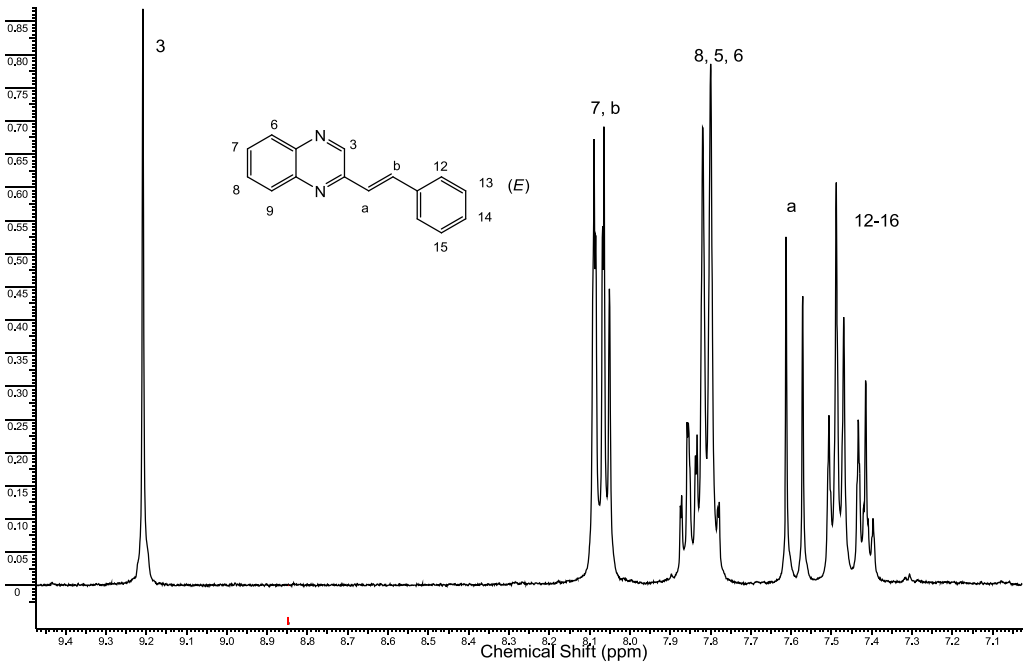


Fig. S5. ^{1}H NMR spectrum of **2**in CD_3CN, Bruker 600 MHz

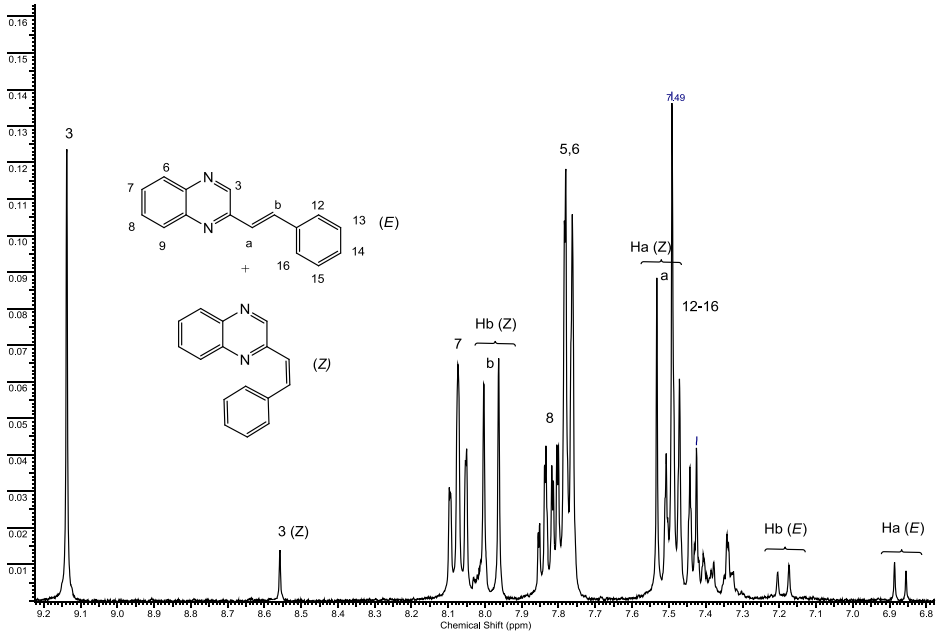


Fig. S6. ^{1}H NMR spectrum of photostationary mixture of **2**+ **2a** in CD_3CN, Bruker 400 MHz

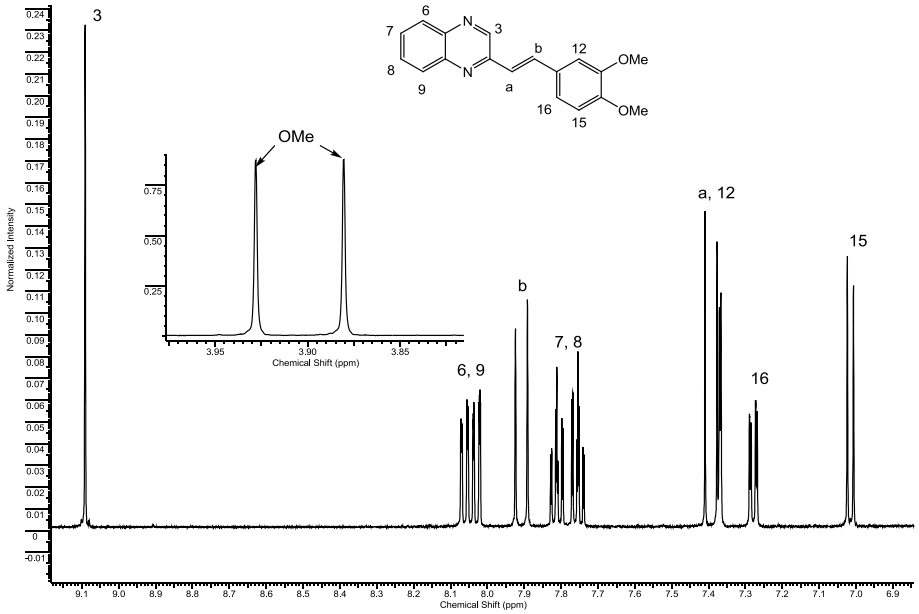


Fig. S7. ^{1}H NMR spectrum of of **1** in CD_3CN, Bruker 600 MHz

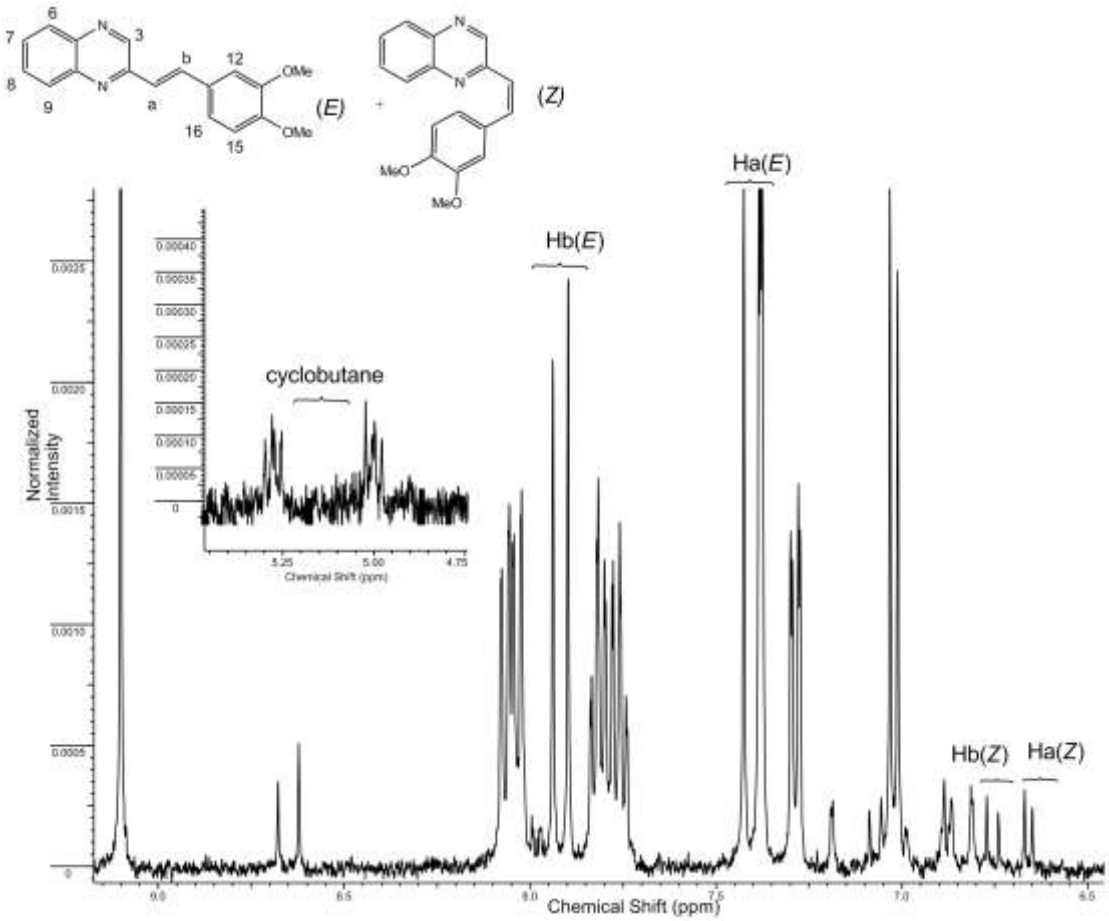


Fig. S8. ^{1}H NMR spectrum of photostationary mixture of **1**+**1a** in CD_3CN, Bruker 400 MHz

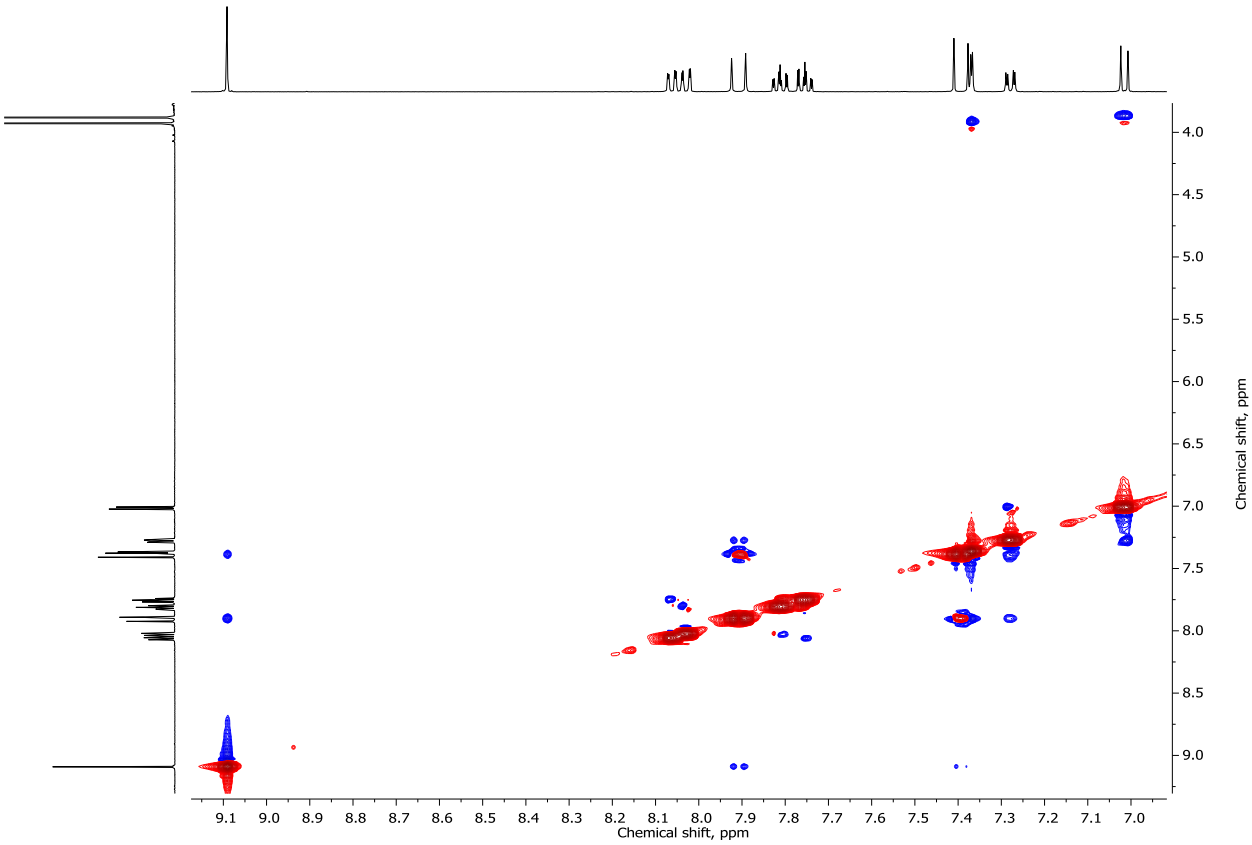


Fig. S9. NOESY spectrum of *E*-**1** in CD_3CN, Bruker 600 MHz

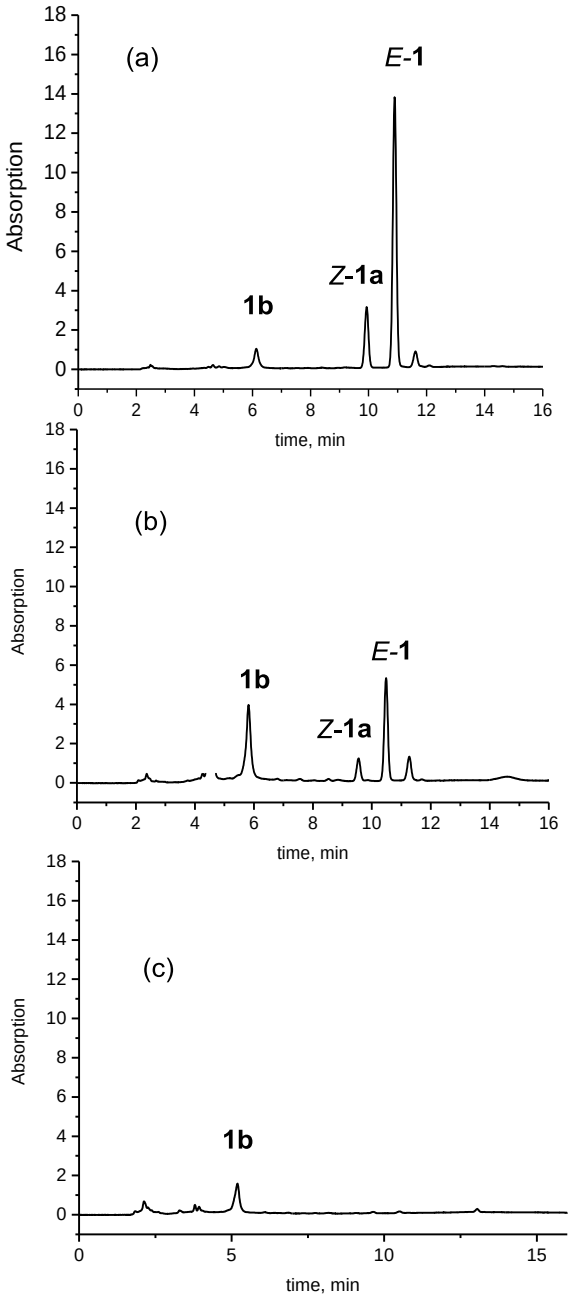


Fig. S10. HPLC of the products of the photolysis of *E*-**1** with full light during (a) 1 minute; (b) 3 minutes; (c) 7 minutes, eluent MeCN:H_2O, 65:35.

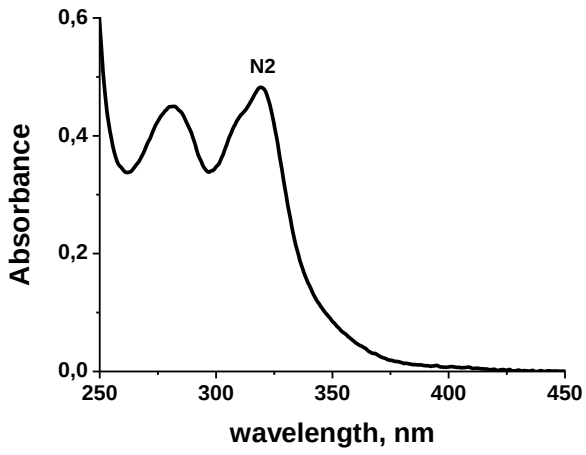


Fig. S11 Cyclobutane (**1b**) absorption spectrum, MeCN, 20°C, $C_{\mathbf{1b}} = 3.9*10^{-5}$ M.

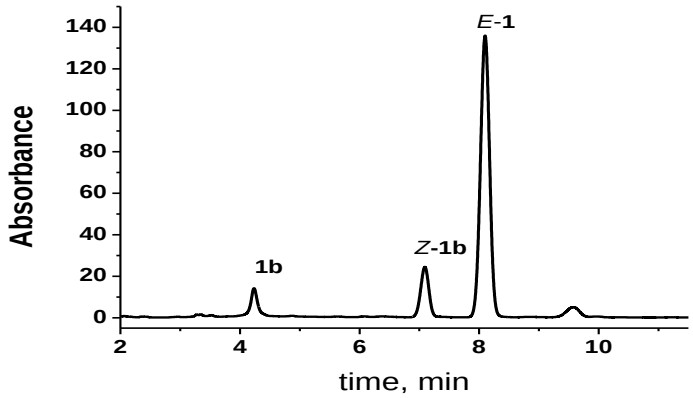


Fig. S12.HPLC of mixture formed in photolysis of **1b** with light 313 nm in MeCN, eluent MeCN:H_2O, 60:40.

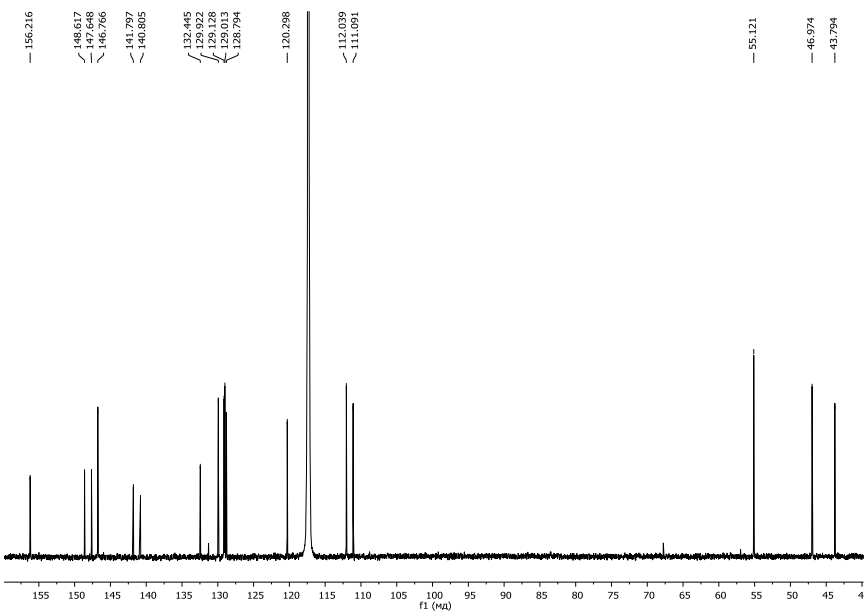


Fig. S13. ^{13}C NMR spectrum of **1b** in CD_3CN, Brucker 600 MHz

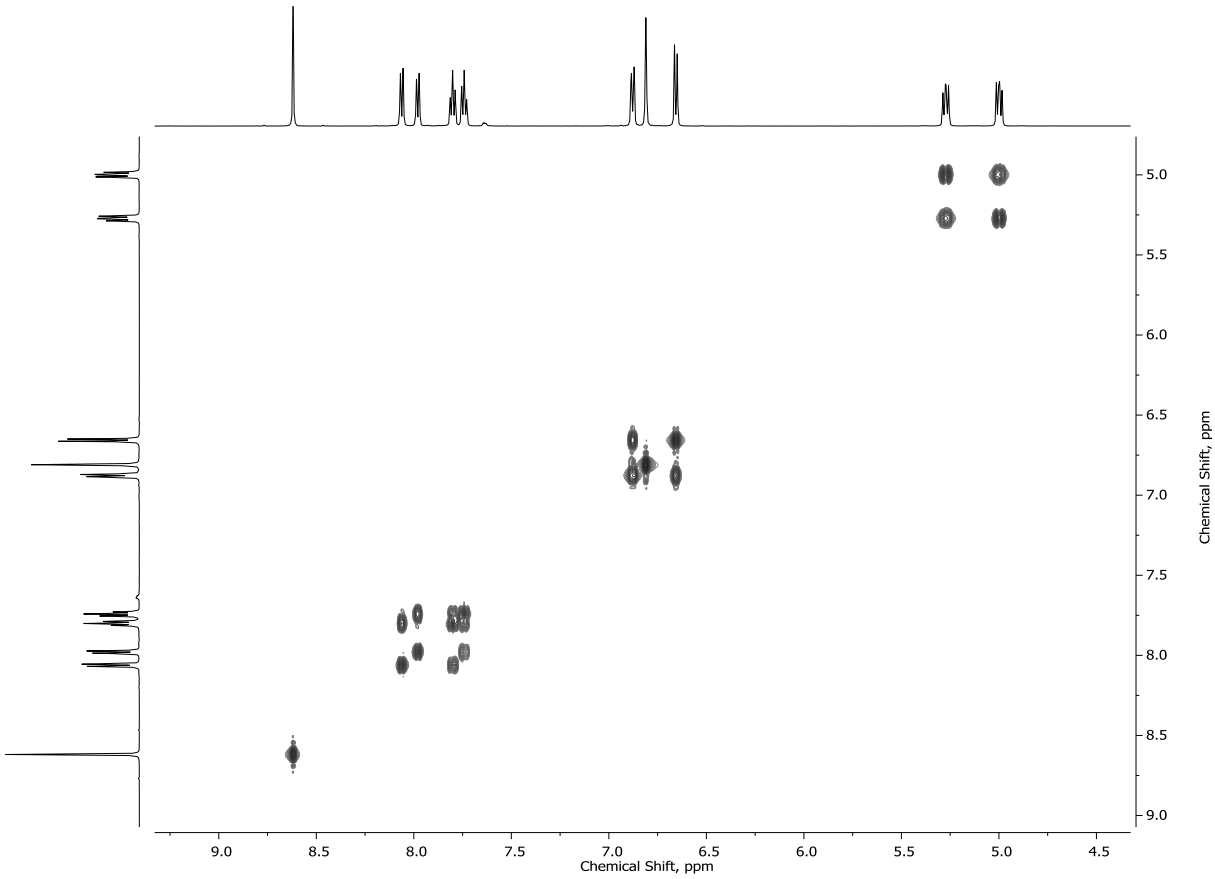


Fig. S14. COSY spectrum of **1b** in CD_3CN, Bruker 600 MHz

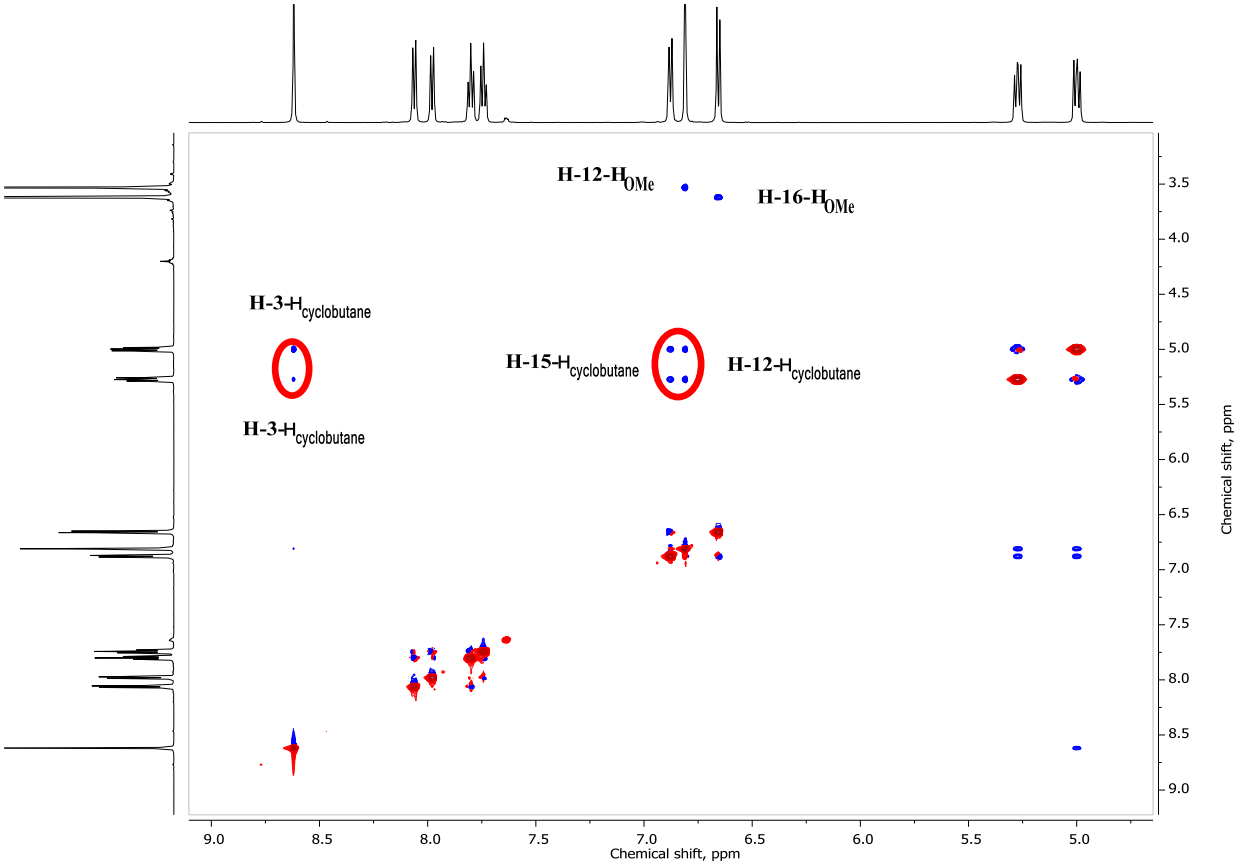


Fig. S15. NOESY spectrum of **1b** in CD_3CN, Bruker 600 MHz

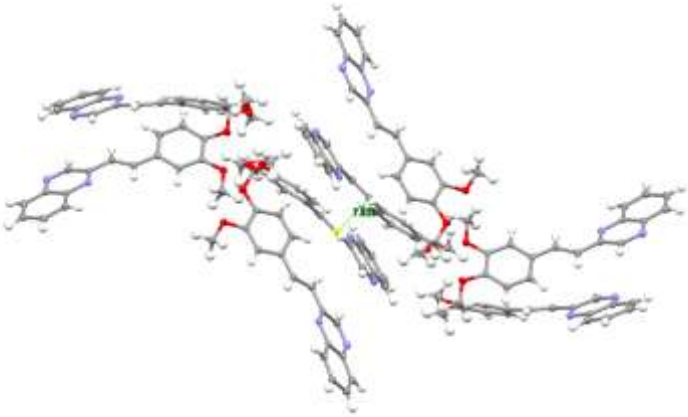
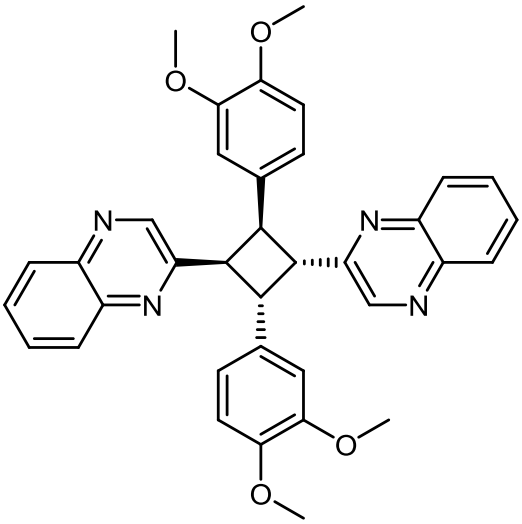
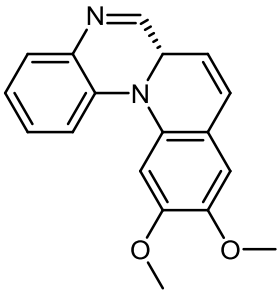


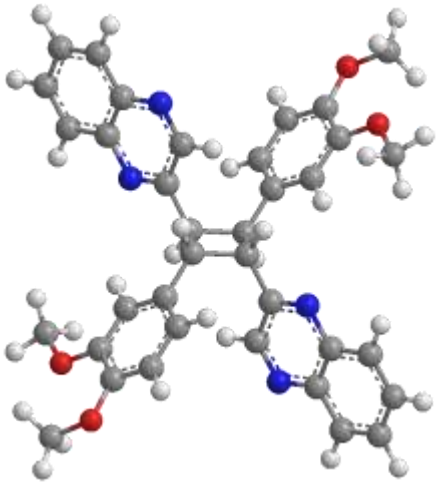
Fig. S16. X-Ray structure of *E*-**1**.



$_{\Delta}H_f$=81 kJ/mol



$_{\Delta}H_f$=136 kJ/mol



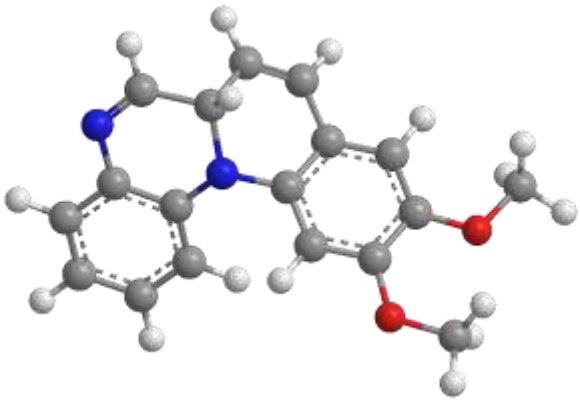


Fig. S17. Optimized geometries (PM6, MOPAC2016) of **1b** and C−N electrocyclic intermediates including calculated standard enthalpy of formation.

C−N electrocyclic intermediate:

ATOM NUMBER	CHEMICAL SYMBOL	X (ANGSTROMS)	Y (ANGSTROMS)	Z (ANGSTROMS)
1	C	1.74068924 *	2.74441283 *	-0.10548137 *
2	C	2.12587386 *	1.46363483 *	0.30898541 *
3	C	3.46293306 *	1.07057125 *	0.28447477 *
4	C	4.45521120 *	1.97210776 *	-0.14629415 *
5	C	4.05395917 *	3.26187777 *	-0.60824058 *
6	C	2.70211679 *	3.63965364 *	-0.57046615 *
7	N	5.85247524 *	1.69432413 *	-0.04733474 *
8	C	6.78944228 *	2.48006146 *	-0.92889257 *
9	C	6.20943308 *	3.83687358 *	-1.29609920 *
10	N	4.98192782 *	4.20165199 *	-1.14202084 *
11	C	6.28856650 *	0.32785645 *	0.14561972 *
12	C	7.03194693 *	-0.33201114 *	-0.85912116 *
13	C	7.31130301 *	0.37559776 *	-2.11087729 *
14	C	7.18759177 *	1.70969465 *	-2.16755551 *
15	C	6.02673848 *	-0.30709868 *	1.37079501 *
16	C	6.48483770 *	-1.60933021 *	1.58916860 *
17	C	7.22403958 *	-2.28259506 *	0.57075321 *
18	C	7.49372861 *	-1.64116206 *	-0.63332239 *
19	O	7.62906855 *	-3.56823258 *	0.89488203 *
20	C	8.35924618 *	-4.30883227 *	-0.11230150 *
21	O	6.13969746 *	-2.08897184 *	2.82679069 *
22	C	6.59512294 *	-3.41355313 *	3.20465992 *
23	H	0.69412014 *	3.03705363 *	-0.07109139 *
24	H	1.36877501 *	0.75881970 *	0.65452002 *
25	H	3.72405114 *	0.06006827 *	0.59541294 *
26	H	2.42027405 *	4.63709056 *	-0.91438739 *
27	H	7.71271173 *	2.64299599 *	-0.29556097 *
28	H	6.92628017 *	4.54421116 *	-1.73397094 *
29	H	7.60726385 *	-0.22370231 *	-2.97013233 *
30	H	7.36424459 *	2.28600604 *	-3.07022096 *
31	H	5.48533272 *	0.21021441 *	2.16672297 *
32	H	8.06453689 *	-2.13871561 *	-1.41445074 *
33	H	8.53640639 *	-5.26288433 *	0.40083838 *
34	H	7.74145189 *	-4.45275259 *	-1.00334945 *
35	H	9.30370120 *	-3.80834699 *	-0.34442711 *
36	H	6.19617304 *	-3.50431593 *	4.22148813 *
37	H	6.16597914 *	-4.16287578 *	2.53085905 *
38	H	7.68934862 *	-3.45329735 *	3.19262788 *

CARTESIAN COORDINATES

1	C	1.740689239	2.744412829	-0.105481372
2	C	2.125873864	1.463634830	0.308985410
3	C	3.462933061	1.070571247	0.284474770
4	C	4.455211203	1.972107761	-0.146294148
5	C	4.053959169	3.261877769	-0.608240584
6	C	2.702116788	3.639653636	-0.570466155
7	N	5.852475240	1.694324128	-0.047334737

8	C	6.789442283	2.480061459	-0.928892568
9	C	6.209433077	3.836873582	-1.296099199
10	N	4.981927817	4.201651989	-1.142020841
11	C	6.288566504	0.327856446	0.145619724
12	C	7.031946932	-0.332011135	-0.859121160
13	C	7.311303010	0.375597758	-2.110877286
14	C	7.187591771	1.709694652	-2.167555509
15	C	6.026738478	-0.307098685	1.370795007
16	C	6.484837701	-1.609330214	1.589168595
17	C	7.224039583	-2.282595057	0.570753212
18	C	7.493728613	-1.641162055	-0.633322393
19	O	7.629068553	-3.568232583	0.894882028
20	C	8.359246177	-4.308832270	-0.112301505
21	O	6.139697462	-2.088971836	2.826790693
22	C	6.595122936	-3.413553126	3.204659918
23	H	0.694120141	3.037053630	-0.071091389
24	H	1.368775006	0.758819702	0.654520022
25	H	3.724051136	0.060068274	0.595412935
26	H	2.420274053	4.637090557	-0.914387386
27	H	7.712711731	2.642995987	-0.295560966
28	H	6.926280172	4.544211157	-1.733970939
29	H	7.607263853	-0.223702310	-2.970132332
30	H	7.364244588	2.286006039	-3.070220963
31	H	5.485332721	0.210214407	2.166722973
32	H	8.064536886	-2.138715611	-1.414450736
33	H	8.536406391	-5.262884326	0.400838378
34	H	7.741451886	-4.452752589	-1.003349452
35	H	9.303701198	-3.808346988	-0.344427110
36	H	6.196173044	-3.504315928	4.221488125
37	H	6.165979138	-4.162875777	2.530859054
38	H	7.689348619	-3.453297348	3.192627884

Empirical Formula: C18 H16 N2 O2 = 38 atoms

BOND ORDERS AND VALENCIES

		C 1	C 2	C 3	C 4	C 5	C 6
C	1	3.966517					
C	2	1.412909	3.969344				
C	3	0.004689	1.455544	3.952815			
C	4	0.092562	0.002415	1.366418	3.946081		
C	5	0.004382	0.097621	0.003759	1.309774	3.960804	
C	6	1.452661	0.002073	0.099003	0.003434	1.387996	3.962373
N	7	0.014554	0.008549	0.034520	1.053784	0.031417	0.006035
C	8	0.001799	0.000997	0.012087	0.012463	0.012377	0.000188
C	9	0.001720	0.016088	0.000292	0.034303	0.013299	0.040606
N	10	0.007691	0.000299	0.006294	0.014473	1.052967	0.003384
C	11	0.001362	0.000192	0.003886	0.009047	0.011764	0.000913
C	12	0.000899	0.000076	0.001896	0.011388	0.001809	0.000175
C	13	0.000140	0.000041	0.000305	0.000613	0.000406	0.000033

C	14	0.000780	0.000137	0.001197	0.001581	0.001847	0.000673
C	15	0.000535	0.000211	0.001726	0.008281	0.001096	0.000150
C	16	0.000048	0.000057	0.000725	0.000314	0.000157	0.000019
C	17	0.000280	0.000034	0.000499	0.003072	0.000506	0.000058
C	18	0.000058	0.000025	0.000302	0.000467	0.000212	0.000020
O	19	0.000045	0.000007	0.000075	0.000505	0.000081	0.000010
C	20	0.000001	0.000000	0.000002	0.000002	0.000001	0.000000
O	21	0.000012	0.000006	0.000097	0.000041	0.000024	0.000002
C	22	0.000000	0.000001	0.000001	0.000024	0.000007	0.000001
H	23	0.961225	0.000558	0.005923	0.000103	0.006183	0.000527
H	24	0.000956	0.964973	0.000936	0.006225	0.000083	0.005902
H	25	0.005874	0.000228	0.951645	0.000962	0.005511	0.000086
H	26	0.000904	0.006045	0.000077	0.006037	0.001186	0.957796
H	27	0.000146	0.000221	0.000335	0.007296	0.000343	0.000463
H	28	0.000221	0.000004	0.000295	0.000013	0.015844	0.000142
H	29	0.000005	0.000004	0.000008	0.000014	0.000015	0.000017
H	30	0.000050	0.000011	0.000142	0.000206	0.000094	0.000000
H	31	0.000002	0.000014	0.000116	0.000171	0.000016	0.000003
H	32	0.000009	0.000001	0.000016	0.000076	0.000022	0.000002
H	33	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	34	0.000001	0.000000	0.000001	0.000009	0.000002	0.000000
H	35	0.000001	0.000000	0.000001	0.000010	0.000001	0.000000
H	36	0.000000	0.000000	0.000000	0.000002	0.000000	0.000000
H	37	0.000000	0.000000	0.000001	0.000000	0.000000	0.000000
H	38	0.000000	0.000000	0.000002	0.000000	0.000000	0.000000

		N 7	C 8	C 9	N 10	C 11	C 12
N	7	3.186657					
C	8	0.927010	3.935459				
C	9	0.008821	0.968617	3.947827			
N	10	0.004048	0.031283	1.901701	3.045138		
C	11	0.998439	0.009279	0.007051	0.000503	3.953430	
C	12	0.022813	0.003310	0.000628	0.000132	1.387227	3.982630
C	13	0.008893	0.004383	0.006633	0.000910	0.002473	1.051754
C	14	0.016291	0.985992	0.002623	0.010346	0.031113	0.003895
C	15	0.015803	0.008699	0.000545	0.000071	1.358750	0.005498
C	16	0.007394	0.001013	0.000167	0.000026	0.002560	0.092121
C	17	0.005284	0.000102	0.000141	0.000027	0.088518	0.009185
C	18	0.006904	0.000230	0.000137	0.000018	0.003035	1.347428
O	19	0.000781	0.000028	0.000026	0.000006	0.013122	0.008854
C	20	0.000031	0.000002	0.000001	0.000000	0.000045	0.000222
O	21	0.000608	0.000224	0.000031	0.000004	0.007820	0.017341
C	22	0.000343	0.000125	0.000012	0.000001	0.001901	0.000055
H	23	0.000124	0.000011	0.000149	0.000174	0.000013	0.000001
H	24	0.000319	0.000184	0.000010	0.000099	0.000001	0.000008
H	25	0.000738	0.000102	0.000022	0.000434	0.000721	0.000007
H	26	0.000311	0.000008	0.000116	0.000918	0.000211	0.000015
H	27	0.003541	0.939884	0.001197	0.007297	0.000746	0.000361
H	28	0.004479	0.004512	0.942019	0.001689	0.000806	0.000017
H	29	0.000111	0.008915	0.000182	0.000232	0.004904	0.001044

H	30	0.003667	0.001501	0.000675	0.000109	0.000054	0.008218
H	31	0.000635	0.000123	0.000008	0.000001	0.000712	0.005370
H	32	0.000356	0.000001	0.000005	0.000001	0.005583	0.000260
H	33	0.000001	0.000000	0.000000	0.000000	0.000011	0.000032
H	34	0.000013	0.000000	0.000001	0.000000	0.000232	0.000018
H	35	0.000012	0.000000	0.000000	0.000000	0.000235	0.000018
H	36	0.000020	0.000010	0.000001	0.000000	0.000178	0.000001
H	37	0.000004	0.000000	0.000000	0.000000	0.000011	0.000277
H	38	0.000005	0.000001	0.000000	0.000000	0.000012	0.000278

		C 13	C 14	C 15	C 16	C 17	C 18
C	13	3.972463					
C	14	1.909924	3.966732				
C	15	0.006194	0.000661	3.941756			
C	16	0.000242	0.011442	1.417194	3.929755		
C	17	0.007324	0.001453	0.008759	1.255781	3.931674	
C	18	0.001908	0.024802	0.087341	0.007909	1.457370	3.966434
O	19	0.000639	0.000265	0.008506	0.024297	1.012770	0.056992
C	20	0.000025	0.000005	0.001739	0.014632	0.007963	0.003765
O	21	0.000229	0.002481	0.049029	1.063190	0.046219	0.009122
C	22	0.000019	0.000004	0.015406	0.008492	0.003748	0.000063
H	23	0.000000	0.000001	0.000003	0.000002	0.000001	0.000001
H	24	0.000003	0.000001	0.000007	0.000000	0.000004	0.000000
H	25	0.000005	0.000000	0.001734	0.000035	0.000005	0.000003
H	26	0.000001	0.000002	0.000013	0.000003	0.000006	0.000004
H	27	0.008702	0.001245	0.000113	0.000128	0.000107	0.000365
H	28	0.000061	0.000085	0.000115	0.000029	0.000005	0.000005
H	29	0.959494	0.000555	0.000223	0.000166	0.000010	0.000520
H	30	0.000380	0.957164	0.000155	0.000009	0.000111	0.000192
H	31	0.000182	0.000030	0.941335	0.001406	0.005587	0.000087
H	32	0.000522	0.000040	0.000033	0.005727	0.001462	0.954143
H	33	0.000005	0.000001	0.000174	0.000245	0.012253	0.000239
H	34	0.000006	0.000004	0.000044	0.000277	0.000488	0.001321
H	35	0.000006	0.000004	0.000041	0.000270	0.000480	0.001300
H	36	0.000004	0.000000	0.000326	0.012066	0.000095	0.000108
H	37	0.000002	0.000044	0.000621	0.000798	0.000997	0.000019
H	38	0.000002	0.000042	0.000624	0.000813	0.000971	0.000018

		O 19	C 20	O 21	C 22	H 23	H 24
O	19	2.088581					
C	20	0.934032	3.869497				
O	21	0.003029	0.000259	2.142293			
C	22	0.003285	0.002932	0.926284	3.857528		
H	23	0.000000	0.000000	0.000000	0.000000	0.975451	
H	24	0.000000	0.000000	0.000000	0.000000	0.000162	0.980292
H	25	0.000001	0.000000	0.000000	0.000001	0.000117	0.000188
H	26	0.000001	0.000000	0.000000	0.000000	0.000158	0.000214
H	27	0.000015	0.000000	0.000026	0.000000	0.000003	0.000009

H	28	0.000001	0.000000	0.000005	0.000003	0.000010	0.000007
H	29	0.000005	0.000000	0.000031	0.000001	0.000000	0.000000
H	30	0.000019	0.000000	0.000007	0.000001	0.000000	0.000001
H	31	0.000321	0.000320	0.001350	0.000334	0.000000	0.000000
H	32	0.001305	0.000997	0.000606	0.000016	0.000000	0.000000
H	33	0.001092	0.960998	0.000018	0.000019	0.000000	0.000000
H	34	0.007720	0.969787	0.000036	0.000007	0.000000	0.000000
H	35	0.007790	0.969762	0.000035	0.000008	0.000000	0.000000
H	36	0.000326	0.000802	0.001145	0.961415	0.000000	0.000000
H	37	0.001440	0.000614	0.006537	0.966248	0.000000	0.000000
H	38	0.001187	0.000556	0.006445	0.966770	0.000000	0.000000

		H 25	H 26	H 27	H 28	H 29	H 30
H	25	0.969042					
H	26	0.000089	0.974133				
H	27	0.000011	0.000001	0.973427			
H	28	0.000001	0.000017	0.000009	0.970559		
H	29	0.000000	0.000000	0.000001	0.000001	0.977049	
H	30	0.000000	0.000000	0.000858	0.000159	0.000192	0.973987
H	31	0.000520	0.000001	0.000001	0.000003	0.000055	0.000000
H	32	0.000000	0.000000	0.000002	0.000000	0.000341	0.000010
H	33	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	34	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	35	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	36	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	37	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	38	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000

		H 31	H 32	H 33	H 34	H 35	H 36
H	31	0.958790					
H	32	0.000064	0.972641				
H	33	0.000011	0.000001	0.975181			
H	34	0.000000	0.000469	0.000037	0.980552		
H	35	0.000000	0.000567	0.000035	0.000073	0.980657	
H	36	0.000012	0.000001	0.000002	0.000003	0.000004	0.976532
H	37	0.000000	0.000001	0.000004	0.000002	0.000001	0.000004
H	38	0.000000	0.000001	0.000003	0.000000	0.000002	0.000007

		H 37	H 38
H	37	0.977629	
H	38	0.000000	0.977742

Compound 1b:

ATOM NUMBER	CHEMICAL SYMBOL	X (ANGSTROMS)	Y (ANGSTROMS)	Z (ANGSTROMS)

1	C	-7.16235090	*	0.71222000	*	-0.21283485	*
2	C	-6.85555554	*	-0.68019678	*	-0.15124147	*
3	C	-5.55534221	*	-1.11652741	*	-0.09392103	*
4	C	-4.49317122	*	-0.15917755	*	-0.09607694	*
5	C	-4.79989340	*	1.23391607	*	-0.16097544	*
6	C	-6.16499678	*	1.65520929	*	-0.21827598	*
7	N	-3.17070275	*	-0.59313712	*	-0.03133057	*
8	C	-2.21165232	*	0.33022817	*	-0.04397726	*
9	C	-2.53359587	*	1.74873847	*	-0.12318622	*
10	N	-3.78119645	*	2.18552313	*	-0.17393485	*
11	C	-0.79605603	*	-0.15070316	*	0.06210438	*
12	C	-0.00085343	*	0.47705006	*	1.25097352	*
13	C	1.05043742	*	1.03054585	*	0.23694480	*
14	C	0.26331636	*	0.38998958	*	-0.95010789	*
15	C	-0.17084505	*	1.29115323	*	-2.06567824	*
16	C	0.52265850	*	2.48514019	*	-2.32940880	*
17	C	0.14574485	*	3.29047375	*	-3.40298002	*
18	C	-0.94108038	*	2.90440678	*	-4.23621398	*
19	C	-1.61724940	*	1.70656168	*	-3.97166844	*
20	C	-1.22772985	*	0.90353275	*	-2.89702227	*
21	O	0.75980167	*	4.48245986	*	-3.74642535	*
22	C	1.89631005	*	4.90157475	*	-2.95145263	*
23	C	0.44452416	*	-0.43800613	*	2.35092405	*
24	C	1.49570564	*	-0.04995759	*	3.18940082	*
25	C	1.89738544	*	-0.86652457	*	4.24925785	*
26	C	1.23922916	*	-2.07896214	*	4.49196004	*
27	C	0.15736283	*	-2.46537920	*	3.65243067	*
28	C	-0.23100681	*	-1.64672818	*	2.59314187	*
29	O	-0.43981950	*	-3.67160618	*	3.97517499	*
30	O	-1.44447022	*	3.57105160	*	-5.32933629	*
31	C	2.47465172	*	0.57595238	*	0.34067716	*
32	C	2.82439391	*	-0.83576376	*	0.42156147	*
33	N	4.08052836	*	-1.24810474	*	0.46768092	*
34	C	5.08055834	*	-0.27705146	*	0.44824128	*
35	C	4.74662295	*	1.10969042	*	0.38196029	*
36	N	3.41578282	*	1.51764305	*	0.32180649	*
37	C	6.45388013	*	-0.67161998	*	0.49987076	*
38	C	7.43270591	*	0.29051282	*	0.48772131	*
39	C	7.09868320	*	1.67662378	*	0.42502573	*
40	C	5.79000140	*	2.08749895	*	0.37310832	*
41	O	1.75333123	*	-2.75852718	*	5.57200727	*
42	C	-0.84880443	*	4.84321997	*	-5.68624502	*
43	C	-1.57271569	*	-4.09152214	*	3.17553431	*
44	C	1.18072048	*	-4.04860277	*	5.90144737	*
45	H	-8.20956553	*	1.01251634	*	-0.25697800	*
46	H	-7.68003815	*	-1.39388384	*	-0.15171605	*
47	H	-5.30060939	*	-2.17586980	*	-0.04848327	*
48	H	-6.37613934	*	2.72515824	*	-0.26764937	*
49	H	-1.72418507	*	2.49054265	*	-0.15857524	*
50	H	-0.78391234	*	-1.26654463	*	0.07824543	*
51	H	-0.55814749	*	1.31749111	*	1.72882147	*
52	H	1.01849085	*	2.14620675	*	0.21892393	*

53	H	0.82332700	*	-0.45754710	*	-1.41230351	*
54	H	1.36496695	*	2.76715740	*	-1.69782524	*
55	H	-2.44623612	*	1.41638560	*	-4.61754827	*
56	H	-1.75801205	*	-0.03099092	*	-2.71357237	*
57	H	2.18509899	*	5.83374991	*	-3.45267760	*
58	H	1.58926023	*	5.08930471	*	-1.91852228	*
59	H	2.69831411	*	4.15931399	*	-3.00858717	*
60	H	2.01219115	*	0.89535028	*	3.02266303	*
61	H	2.72213669	*	-0.57586933	*	4.90035538	*
62	H	-1.06874527	*	-1.92974220	*	1.95585069	*
63	H	2.02963420	*	-1.59312397	*	0.46176376	*
64	H	6.68597672	*	-1.73716487	*	0.55041281	*
65	H	8.48575932	*	0.01069656	*	0.52728820	*
66	H	7.90916127	*	2.40617555	*	0.42033010	*
67	H	5.51448216	*	3.14158075	*	0.32726018	*
68	H	-1.44989564	*	5.13676716	*	-6.55401729	*
69	H	-0.95537474	*	5.55393604	*	-4.86008968	*
70	H	0.20460911	*	4.70266281	*	-5.95068218	*
71	H	-1.85014983	*	-5.03435528	*	3.66320861	*
72	H	-2.38320988	*	-3.35956310	*	3.24480089	*
73	H	-1.26469037	*	-4.26046325	*	2.13970076	*
74	H	1.78915172	*	-4.35103313	*	6.76100368	*
75	H	0.12573896	*	-3.93199448	*	6.17130644	*
76	H	1.29716351	*	-4.73886845	*	5.05943002	*

CARTESIAN COORDINATES

1	C	-7.162350900	0.712219996	-0.212834853
2	C	-6.855555538	-0.680196781	-0.151241470
3	C	-5.555342212	-1.116527409	-0.093921027
4	C	-4.493171218	-0.159177552	-0.096076943
5	C	-4.799893401	1.233916065	-0.160975438
6	C	-6.164996777	1.655209288	-0.218275977
7	N	-3.170702750	-0.593137118	-0.031330572
8	C	-2.211652323	0.330228168	-0.043977264
9	C	-2.533595869	1.748738474	-0.123186217
10	N	-3.781196448	2.185523128	-0.173934849
11	C	-0.796056025	-0.150703161	0.062104381
12	C	-0.000853434	0.477050056	1.250973519
13	C	1.050437421	1.030545852	0.236944796
14	C	0.263316357	0.389989575	-0.950107893
15	C	-0.170845048	1.291153227	-2.065678236
16	C	0.522658500	2.485140194	-2.329408799
17	C	0.145744852	3.290473753	-3.402980019
18	C	-0.941080380	2.904406782	-4.236213981
19	C	-1.617249398	1.706561685	-3.971668441
20	C	-1.227729848	0.903532747	-2.897022265
21	O	0.759801674	4.482459856	-3.746425353
22	C	1.896310045	4.901574747	-2.951452631
23	C	0.444524157	-0.438006129	2.350924047
24	C	1.495705639	-0.049957586	3.189400815
25	C	1.897385442	-0.866524568	4.249257846

26	C	1.239229157	-2.078962138	4.491960044
27	C	0.157362832	-2.465379197	3.652430667
28	C	-0.231006814	-1.646728176	2.593141871
29	O	-0.439819498	-3.671606179	3.975174988
30	O	-1.444470224	3.571051597	-5.329336292
31	C	2.474651722	0.575952382	0.340677157
32	C	2.824393906	-0.835763763	0.421561468
33	N	4.080528355	-1.248104740	0.467680920
34	C	5.080558340	-0.277051461	0.448241278
35	C	4.746622952	1.109690425	0.381960289
36	N	3.415782821	1.517643051	0.321806494
37	C	6.453880132	-0.671619983	0.499870757
38	C	7.432705910	0.290512821	0.487721314
39	C	7.098683200	1.676623782	0.425025732
40	C	5.790001401	2.087498948	0.373108323
41	O	1.753331227	-2.758527182	5.572007272
42	C	-0.848804431	4.843219971	-5.686245017
43	C	-1.572715694	-4.091522144	3.175534307
44	C	1.180720479	-4.048602767	5.901447367
45	H	-8.209565527	1.012516344	-0.256978000
46	H	-7.680038152	-1.393883840	-0.151716048
47	H	-5.300609385	-2.175869800	-0.048483269
48	H	-6.376139337	2.725158243	-0.267649370
49	H	-1.724185071	2.490542646	-0.158575237
50	H	-0.783912338	-1.266544629	0.078245435
51	H	-0.558147488	1.317491106	1.728821465
52	H	1.018490849	2.146206752	0.218923931
53	H	0.823326998	-0.457547103	-1.412303507
54	H	1.364966946	2.767157403	-1.697825235
55	H	-2.446236116	1.416385596	-4.617548269
56	H	-1.758012053	-0.030990920	-2.713572370
57	H	2.185098992	5.833749911	-3.452677601
58	H	1.589260229	5.089304708	-1.918522277
59	H	2.698314106	4.159313995	-3.008587174
60	H	2.012191151	0.895350278	3.022663033
61	H	2.722136685	-0.575869333	4.900355380
62	H	-1.068745271	-1.929742202	1.955850687
63	H	2.029634202	-1.593123973	0.461763761
64	H	6.685976719	-1.737164875	0.550412809
65	H	8.485759318	0.010696557	0.527288200
66	H	7.909161268	2.406175550	0.420330104
67	H	5.514482163	3.141580748	0.327260176
68	H	-1.449895643	5.136767164	-6.554017292
69	H	-0.955374737	5.553936036	-4.860089682
70	H	0.204609107	4.702662808	-5.950682182
71	H	-1.850149831	-5.034355279	3.663208615
72	H	-2.383209879	-3.359563101	3.244800886
73	H	-1.264690370	-4.260463248	2.139700765
74	H	1.789151715	-4.351033127	6.761003680
75	H	0.125738957	-3.931994485	6.171306437
76	H	1.297163515	-4.738868450	5.059430021

Empirical Formula: C36 H32 N4 O4 = 76 atoms

BOND ORDERS AND VALENCIES

		C 1	C 2	C 3	C 4	C 5	C 6
C	1	3.972294					
C	2	1.249293	3.972282				
C	3	0.001555	1.639126	3.967023			
C	4	0.069177	0.002225	1.215199	3.971190		
C	5	0.002132	0.069021	0.004058	1.331809	3.975586	
C	6	1.639391	0.001738	0.101455	0.003953	1.214944	3.965138
N	7	0.000173	0.018914	0.003928	1.210326	0.016282	0.008678
C	8	0.019975	0.001099	0.029884	0.007546	0.085216	0.000084
C	9	0.001051	0.020083	0.000112	0.083040	0.009763	0.030416
N	10	0.018696	0.000314	0.008714	0.016498	1.211268	0.003604
C	11	0.000039	0.000201	0.000204	0.015707	0.000267	0.000375
C	12	0.000552	0.000031	0.000535	0.000609	0.001893	0.000015
C	13	0.000013	0.000003	0.000014	0.000148	0.000046	0.000004
C	14	0.000461	0.000026	0.000477	0.000767	0.001570	0.000004
C	15	0.000007	0.000018	0.000009	0.000080	0.000020	0.000012
C	16	0.000005	0.000004	0.000005	0.000020	0.000023	0.000003
C	17	0.000004	0.000006	0.000003	0.000020	0.000010	0.000004
C	18	0.000001	0.000004	0.000001	0.000013	0.000006	0.000004
C	19	0.000009	0.000006	0.000006	0.000020	0.000033	0.000004
C	20	0.000017	0.000012	0.000014	0.000041	0.000070	0.000017
O	21	0.000001	0.000001	0.000001	0.000003	0.000002	0.000001
C	22	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	23	0.000013	0.000002	0.000013	0.000054	0.000047	0.000002
C	24	0.000010	0.000001	0.000009	0.000009	0.000033	0.000000
C	25	0.000001	0.000000	0.000001	0.000002	0.000004	0.000000
C	26	0.000000	0.000000	0.000000	0.000001	0.000001	0.000000
C	27	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	28	0.000002	0.000001	0.000002	0.000011	0.000006	0.000001
O	29	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
O	30	0.000000	0.000001	0.000000	0.000003	0.000002	0.000001
C	31	0.000000	0.000000	0.000001	0.000013	0.000001	0.000000
C	32	0.000001	0.000000	0.000000	0.000000	0.000002	0.000000
N	33	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	34	0.000001	0.000000	0.000001	0.000000	0.000002	0.000000
C	35	0.000000	0.000000	0.000000	0.000002	0.000000	0.000000
N	36	0.000003	0.000000	0.000002	0.000003	0.000008	0.000000
C	37	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	38	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
C	39	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	40	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
O	41	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	42	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

C 1 C 2 C 3 C 4 C 5 C 6

C	43	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	44	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	45	0.961182	0.000762	0.005141	0.000078	0.007082	0.000638
H	46	0.000788	0.961866	0.000693	0.007076	0.000073	0.005135
H	47	0.006872	0.000637	0.955476	0.000902	0.005419	0.000059
H	48	0.000705	0.006875	0.000057	0.005429	0.000912	0.954495
H	49	0.000153	0.000003	0.000285	0.000085	0.013484	0.000099
H	50	0.000001	0.000005	0.000030	0.000225	0.000030	0.000000
H	51	0.000000	0.000001	0.000001	0.000021	0.000001	0.000001
H	52	0.000000	0.000000	0.000001	0.000007	0.000000	0.000000
H	53	0.000007	0.000001	0.000007	0.000062	0.000026	0.000001
H	54	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	55	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	56	0.000002	0.000000	0.000002	0.000006	0.000012	0.000001
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	60	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	61	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
H	62	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	63	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	71	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	75	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	76	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

		N 7	C 8	C 9	N 10	C 11	C 12
N	7	3.015519					
C	8	1.632658	3.957433				
C	9	0.020362	1.147578	3.942065			
N	10	0.068392	0.021525	1.673079	3.033400		
C	11	0.005411	0.991851	0.006460	0.006661	3.963891	
C	12	0.010744	0.002970	0.002721	0.000313	0.976742	3.970896
C	13	0.000280	0.002501	0.000167	0.000033	0.001207	0.971575
C	14	0.010011	0.002772	0.002116	0.000094	0.971786	0.000797
C	15	0.000213	0.001012	0.000402	0.000274	0.001932	0.002771
C	16	0.000068	0.000108	0.000294	0.000056	0.007022	0.000287
C	17	0.000054	0.000029	0.000014	0.000067	0.000236	0.000019
C	18	0.000012	0.000013	0.000084	0.000046	0.001408	0.000025
C	19	0.000116	0.000028	0.000039	0.000083	0.000061	0.000030

C	20	0.000460	0.000295	0.000866	0.000266	0.004176	0.000162
O	21	0.000012	0.000004	0.000003	0.000013	0.000115	0.000004
C	22	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
C	23	0.000212	0.002256	0.000063	0.000029	0.001537	0.999800
C	24	0.000147	0.000124	0.000041	0.000006	0.006148	0.003833
C	25	0.000017	0.000048	0.000004	0.000001	0.000360	0.007124
C	26	0.000003	0.000002	0.000005	0.000002	0.000239	0.000590
C	27	0.000002	0.000018	0.000003	0.000000	0.000261	0.006768
C	28	0.000049	0.000033	0.000032	0.000007	0.004026	0.003897
O	29	0.000000	0.000001	0.000001	0.000000	0.000045	0.000633
O	30	0.000003	0.000003	0.000018	0.000008	0.000265	0.000002
C	31	0.000028	0.000047	0.000012	0.000001	0.002667	0.002777
C	32	0.000007	0.000009	0.000006	0.000001	0.000136	0.002118
N	33	0.000001	0.000001	0.000001	0.000000	0.000034	0.000093
C	34	0.000008	0.000001	0.000002	0.000000	0.000046	0.001570
C	35	0.000003	0.000012	0.000000	0.000000	0.000154	0.000773
N	36	0.000032	0.000027	0.000007	0.000001	0.000291	0.010013
C	37	0.000000	0.000000	0.000000	0.000000	0.000004	0.000004
C	38	0.000003	0.000000	0.000001	0.000000	0.000013	0.000461
C	39	0.000000	0.000000	0.000000	0.000000	0.000003	0.000026
C	40	0.000002	0.000001	0.000000	0.000000	0.000014	0.000477
O	41	0.000001	0.000001	0.000001	0.000000	0.000045	0.000232
C	42	0.000001	0.000000	0.000000	0.000000	0.000001	0.000000
C	43	0.000000	0.000000	0.000000	0.000000	0.000009	0.000027
C	44	0.000000	0.000000	0.000000	0.000000	0.000002	0.000023
H	45	0.000095	0.000006	0.000194	0.000200	0.000009	0.000000
H	46	0.000214	0.000200	0.000005	0.000094	0.000013	0.000002
H	47	0.000670	0.000075	0.000020	0.000415	0.000026	0.000001
H	48	0.000426	0.000020	0.000076	0.000673	0.000004	0.000000
H	49	0.005104	0.002413	0.937612	0.001571	0.000039	0.000048
H	50	0.001162	0.000820	0.004779	0.000349	0.953049	0.000293
H	51	0.000043	0.000934	0.000457	0.000014	0.000491	0.954043
H	52	0.000012	0.000061	0.000003	0.000001	0.001130	0.000174

		N 7	C 8	C 9	N 10	C 11	C 12
H	53	0.000114	0.002510	0.000062	0.000009	0.000287	0.000863
H	54	0.000001	0.000002	0.000001	0.000000	0.000040	0.000002
H	55	0.000000	0.000001	0.000001	0.000000	0.000003	0.000002
H	56	0.000007	0.000625	0.000006	0.000016	0.000101	0.000008
H	57	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	60	0.000001	0.000003	0.000000	0.000000	0.000037	0.000489
H	61	0.000003	0.000004	0.000001	0.000000	0.000079	0.000253
H	62	0.000048	0.000025	0.000001	0.000000	0.000377	0.000604
H	63	0.000000	0.000000	0.000000	0.000000	0.000033	0.000050
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000003
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000002

H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000005	0.000000
H	70	0.000000	0.000000	0.000000	0.000000	0.000004	0.000000
H	71	0.000000	0.000000	0.000000	0.000000	0.000000	0.000006
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000003
H	73	0.000000	0.000000	0.000000	0.000000	0.000001	0.000003
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000006
H	75	0.000000	0.000000	0.000000	0.000000	0.000001	0.000001
H	76	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001

		C 13	C 14	C 15	C 16	C 17	C 18
C	13	3.963824					
C	14	0.976692	3.970921				
C	15	0.001560	0.999759	3.986238			
C	16	0.003782	0.003896	1.378141	3.953760		
C	17	0.000252	0.006762	0.005127	1.426432	3.930591	
C	18	0.000258	0.000594	0.101823	0.006432	1.281106	3.934082
C	19	0.000359	0.007128	0.002549	0.093895	0.011790	1.413721
C	20	0.006177	0.003846	1.448799	0.003392	0.096827	0.003369
O	21	0.000044	0.000632	0.008336	0.055082	1.020420	0.027779
C	22	0.000009	0.000027	0.000234	0.003923	0.007970	0.014860
C	23	0.001932	0.002620	0.000033	0.000043	0.000001	0.000014
C	24	0.004282	0.000156	0.000035	0.000006	0.000000	0.000001
C	25	0.000060	0.000029	0.000000	0.000001	0.000000	0.000000
C	26	0.001460	0.000025	0.000014	0.000002	0.000000	0.000000
C	27	0.000231	0.000018	0.000001	0.000001	0.000000	0.000000
C	28	0.007043	0.000283	0.000044	0.000011	0.000001	0.000002
O	29	0.000113	0.000004	0.000000	0.000000	0.000000	0.000000
O	30	0.000049	0.000232	0.017976	0.008392	0.047167	1.045131
C	31	0.991930	0.003000	0.002170	0.000038	0.000018	0.000003
C	32	0.006457	0.002749	0.000063	0.000031	0.000003	0.000005
N	33	0.006662	0.000314	0.000028	0.000007	0.000000	0.000002
C	34	0.000267	0.001904	0.000046	0.000007	0.000000	0.000001
C	35	0.015695	0.000609	0.000051	0.000014	0.000000	0.000001
N	36	0.005414	0.010773	0.000205	0.000058	0.000002	0.000003
C	37	0.000375	0.000015	0.000002	0.000001	0.000000	0.000000
C	38	0.000039	0.000555	0.000013	0.000002	0.000000	0.000000
C	39	0.000200	0.000031	0.000002	0.000001	0.000000	0.000000
C	40	0.000204	0.000537	0.000012	0.000002	0.000000	0.000000
O	41	0.000275	0.000002	0.000003	0.000000	0.000000	0.000000
C	42	0.000002	0.000023	0.000035	0.000060	0.003670	0.008311
C	43	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
C	44	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
H	45	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	46	0.000000	0.000003	0.000000	0.000000	0.000000	0.000000
H	47	0.000000	0.000002	0.000000	0.000000	0.000000	0.000000
H	48	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	49	0.000042	0.000051	0.000577	0.000080	0.000005	0.000002
H	50	0.001229	0.000176	0.002057	0.000048	0.000029	0.000005
H	51	0.000286	0.000949	0.000072	0.000008	0.000002	0.000003

H	52	0.953230	0.000286	0.000765	0.000484	0.000008	0.000004
H	53	0.000488	0.953937	0.001449	0.004731	0.000034	0.001740
H	54	0.000377	0.000599	0.000261	0.947955	0.001367	0.005484
H	55	0.000079	0.000253	0.005802	0.000062	0.005669	0.001556
H	56	0.000036	0.000489	0.000814	0.005956	0.000130	0.005984
H	57	0.000000	0.000006	0.000029	0.000256	0.012116	0.000256
H	58	0.000000	0.000003	0.000007	0.001245	0.000534	0.000317

		C 13	C 14	C 15	C 16	C 17	C 18
H	59	0.000000	0.000003	0.000009	0.001260	0.000579	0.000315
H	60	0.000096	0.000007	0.000000	0.000000	0.000000	0.000000
H	61	0.000003	0.000001	0.000000	0.000000	0.000000	0.000000
H	62	0.000039	0.000002	0.000001	0.000000	0.000000	0.000000
H	63	0.000039	0.000047	0.000002	0.000000	0.000000	0.000000
H	64	0.000003	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000009	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000013	0.000002	0.000000	0.000000	0.000000	0.000000
H	67	0.000026	0.000001	0.000000	0.000000	0.000000	0.000000
H	68	0.000000	0.000006	0.000002	0.000109	0.000087	0.012081
H	69	0.000001	0.000001	0.000287	0.000008	0.001007	0.000661
H	70	0.000001	0.000001	0.000290	0.000009	0.001012	0.000640
H	71	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	75	0.000004	0.000000	0.000000	0.000000	0.000000	0.000000
H	76	0.000005	0.000000	0.000000	0.000000	0.000000	0.000000

		C 19	C 20	O 21	C 22	C 23	C 24
C	19	3.963689					
C	20	1.406757	3.969579				
O	21	0.009601	0.014694	2.095677			
C	22	0.001719	0.000054	0.931723	3.867110		
C	23	0.000000	0.000035	0.000000	0.000000	3.986227	
C	24	0.000001	0.000006	0.000000	0.000000	1.448576	3.969603
C	25	0.000000	0.000001	0.000000	0.000000	0.002545	1.406913
C	26	0.000000	0.000001	0.000000	0.000000	0.101821	0.003363
C	27	0.000000	0.000000	0.000000	0.000000	0.005151	0.096829
C	28	0.000001	0.000006	0.000000	0.000000	1.378247	0.003398
O	29	0.000000	0.000000	0.000000	0.000000	0.008336	0.014695
O	30	0.045244	0.007761	0.003332	0.000259	0.000002	0.000000
C	31	0.000046	0.000121	0.000001	0.000000	0.001007	0.000284
C	32	0.000004	0.000042	0.000001	0.000000	0.000410	0.000912
N	33	0.000001	0.000006	0.000000	0.000000	0.000283	0.000272
C	34	0.000004	0.000033	0.000000	0.000000	0.000020	0.000071
C	35	0.000002	0.000009	0.000000	0.000000	0.000083	0.000041
N	36	0.000017	0.000147	0.000000	0.000001	0.000207	0.000446
C	37	0.000000	0.000000	0.000000	0.000000	0.000013	0.000017

C	38	0.000001	0.000011	0.000000	0.000000	0.000007	0.000017
C	39	0.000000	0.000001	0.000000	0.000000	0.000019	0.000012
C	40	0.000001	0.000010	0.000000	0.000000	0.000009	0.000014
O	41	0.000000	0.000000	0.000000	0.000000	0.017988	0.007762
C	42	0.015167	0.002042	0.003145	0.002835	0.000000	0.000000
C	43	0.000000	0.000000	0.000000	0.000000	0.000234	0.000054
C	44	0.000000	0.000000	0.000000	0.000000	0.000036	0.002041
H	45	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	46	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	47	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	48	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	49	0.000006	0.000009	0.000001	0.000000	0.000002	0.000000
H	50	0.000021	0.000018	0.000005	0.000000	0.000772	0.000041
H	51	0.000001	0.000012	0.000000	0.000000	0.001445	0.004275
H	52	0.000011	0.000040	0.000002	0.000001	0.002127	0.000020
H	53	0.000003	0.004340	0.000017	0.000001	0.000064	0.000011
H	54	0.000095	0.005432	0.001335	0.001053	0.000001	0.000000
H	55	0.952868	0.000374	0.000388	0.000347	0.000000	0.000000
H	56	0.000480	0.958090	0.000139	0.000026	0.000000	0.000000
H	57	0.000174	0.000011	0.001063	0.961683	0.000000	0.000000
H	58	0.000059	0.000262	0.007576	0.969620	0.000000	0.000000
H	59	0.000060	0.000255	0.007397	0.968878	0.000000	0.000000
H	60	0.000000	0.000000	0.000000	0.000000	0.000813	0.958145
H	61	0.000000	0.000000	0.000000	0.000000	0.005804	0.000374
H	62	0.000000	0.000000	0.000000	0.000000	0.000260	0.005437
H	63	0.000000	0.000000	0.000000	0.000000	0.000612	0.000012
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

		C 19	C 20	O 21	C 22	C 23	C 24
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000323	0.000181	0.000308	0.000762	0.000000	0.000000
H	69	0.000576	0.000007	0.001148	0.000543	0.000000	0.000000
H	70	0.000570	0.000006	0.001348	0.000582	0.000000	0.000000
H	71	0.000000	0.000000	0.000000	0.000000	0.000029	0.000011
H	72	0.000000	0.000000	0.000000	0.000000	0.000009	0.000254
H	73	0.000000	0.000000	0.000000	0.000000	0.000008	0.000262
H	74	0.000000	0.000000	0.000000	0.000000	0.000003	0.000180
H	75	0.000000	0.000000	0.000000	0.000000	0.000291	0.000006
H	76	0.000000	0.000000	0.000000	0.000000	0.000286	0.000007

		C 25	C 26	C 27	C 28	O 29	O 30
C	25	3.963689					
C	26	1.413579	3.934129				
C	27	0.011827	1.281132	3.930607			
C	28	0.093858	0.006415	1.426243	3.953827		
O	29	0.009610	0.027784	1.020460	0.055083	2.095768	

O	30	0.000000	0.000000	0.000000	0.000000	0.000000	2.122437
C	31	0.000029	0.000013	0.000030	0.000107	0.000004	0.000001
C	32	0.000038	0.000088	0.000014	0.000312	0.000003	0.000001
N	33	0.000089	0.000045	0.000070	0.000055	0.000013	0.000000
C	34	0.000033	0.000007	0.000010	0.000024	0.000002	0.000000
C	35	0.000021	0.000013	0.000021	0.000019	0.000003	0.000000
N	36	0.000114	0.000013	0.000052	0.000070	0.000012	0.000001
C	37	0.000005	0.000004	0.000005	0.000003	0.000001	0.000000
C	38	0.000008	0.000001	0.000003	0.000005	0.000001	0.000000
C	39	0.000006	0.000004	0.000007	0.000003	0.000001	0.000000
C	40	0.000005	0.000001	0.000003	0.000006	0.000001	0.000000
O	41	0.045248	1.045284	0.047201	0.008387	0.003335	0.000000
C	42	0.000000	0.000000	0.000000	0.000000	0.000000	0.929300
C	43	0.001720	0.014866	0.007980	0.003918	0.931736	0.000000
C	44	0.015164	0.008314	0.003677	0.000060	0.003151	0.000000
H	45	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	46	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	47	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	48	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	49	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	50	0.000011	0.000004	0.000009	0.000502	0.000002	0.000002
H	51	0.000004	0.001724	0.000035	0.004752	0.000018	0.000001
H	52	0.000021	0.000005	0.000030	0.000050	0.000005	0.000001
H	53	0.000001	0.000002	0.000002	0.000008	0.000000	0.000308
H	54	0.000000	0.000000	0.000000	0.000000	0.000000	0.000515
H	55	0.000000	0.000000	0.000000	0.000000	0.000000	0.001303
H	56	0.000000	0.000000	0.000000	0.000000	0.000000	0.000257
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000018
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000041
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000039
H	60	0.000480	0.005986	0.000130	0.005955	0.000139	0.000000
H	61	0.952842	0.001555	0.005669	0.000062	0.000388	0.000000
H	62	0.000095	0.005486	0.001366	0.947852	0.001336	0.000000
H	63	0.000006	0.000002	0.000005	0.000088	0.000001	0.000000
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.001080
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.006809
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.006908

		C 25	C 26	C 27	C 28	O 29	O 30
H	71	0.000174	0.000255	0.012118	0.000256	0.001065	0.000000
H	72	0.000061	0.000315	0.000583	0.001262	0.007389	0.000000
H	73	0.000059	0.000318	0.000531	0.001241	0.007588	0.000000
H	74	0.000323	0.012080	0.000088	0.000109	0.000309	0.000000
H	75	0.000570	0.000639	0.001013	0.000009	0.001359	0.000000
H	76	0.000576	0.000665	0.001008	0.000008	0.001141	0.000000

		C 31	C 32	N 33	C 34	C 35	N 36
C	31	3.957374					
C	32	1.147818	3.941910				
N	33	0.021535	1.672793	3.033395			
C	34	0.085264	0.009760	1.211453	3.975597		
C	35	0.007562	0.083047	0.016501	1.331769	3.971207	
N	36	1.632191	0.020339	0.068439	0.016278	1.210560	3.015363
C	37	0.000084	0.030404	0.003605	1.214803	0.003950	0.008679
C	38	0.019976	0.001050	0.018707	0.002135	0.069141	0.000173
C	39	0.001103	0.020075	0.000314	0.068979	0.002219	0.018922
C	40	0.029878	0.000112	0.008717	0.004057	1.215035	0.003931
O	41	0.000003	0.000019	0.000007	0.000002	0.000003	0.000003
C	42	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	43	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
C	44	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
H	45	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	46	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	47	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	48	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	49	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	50	0.000069	0.000003	0.000001	0.000000	0.000008	0.000013
H	51	0.002434	0.000061	0.000009	0.000026	0.000060	0.000111
H	52	0.000825	0.004783	0.000349	0.000030	0.000227	0.001174
H	53	0.000925	0.000459	0.000014	0.000001	0.000020	0.000042
H	54	0.000033	0.000001	0.000000	0.000000	0.000000	0.000062
H	55	0.000004	0.000001	0.000000	0.000001	0.000000	0.000003
H	56	0.000003	0.000000	0.000000	0.000000	0.000000	0.000001
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	60	0.000603	0.000007	0.000016	0.000012	0.000006	0.000007
H	61	0.000001	0.000001	0.000000	0.000000	0.000000	0.000000
H	62	0.000002	0.000001	0.000000	0.000000	0.000000	0.000001
H	63	0.002409	0.937467	0.001570	0.013480	0.000085	0.005106
H	64	0.000020	0.000076	0.000673	0.000912	0.005428	0.000425
H	65	0.000006	0.000194	0.000200	0.007083	0.000078	0.000095
H	66	0.000200	0.000005	0.000094	0.000073	0.007077	0.000214
H	67	0.000075	0.000020	0.000415	0.005419	0.000901	0.000670
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	71	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	75	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	76	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

	C 37	C 38	C 39	C 40	O 41	C 42

C	37	3.965125					
C	38	1.639544	3.972285				
C	39	0.001740	1.249160	3.972275			
C	40	0.101449	0.001554	1.639296	3.967044		
O	41	0.000001	0.000000	0.000001	0.000000	2.122613	
C	42	0.000000	0.000000	0.000000	0.000000	0.000000	3.861904
C	43	0.000000	0.000000	0.000000	0.000000	0.000259	0.000000
C	44	0.000000	0.000000	0.000000	0.000000	0.929273	0.000000
H	45	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	46	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	47	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	48	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	49	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	50	0.000000	0.000000	0.000000	0.000001	0.000001	0.000000
H	51	0.000001	0.000007	0.000001	0.000007	0.000305	0.000000
H	52	0.000000	0.000001	0.000005	0.000030	0.000002	0.000000
H	53	0.000001	0.000000	0.000001	0.000001	0.000000	0.000000
H	54	0.000000	0.000000	0.000000	0.000000	0.000000	0.000019
H	55	0.000000	0.000000	0.000000	0.000000	0.000000	0.000276
H	56	0.000000	0.000000	0.000000	0.000000	0.000000	0.000292
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000019
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000007
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000007
H	60	0.000001	0.000002	0.000000	0.000002	0.000256	0.000000
H	61	0.000000	0.000000	0.000000	0.000000	0.001302	0.000000
H	62	0.000000	0.000000	0.000000	0.000000	0.000516	0.000000
H	63	0.000099	0.000153	0.000003	0.000285	0.000000	0.000000
H	64	0.954486	0.000705	0.006876	0.000057	0.000000	0.000000
H	65	0.000638	0.961173	0.000762	0.005140	0.000000	0.000000
H	66	0.005135	0.000788	0.961863	0.000694	0.000000	0.000000
H	67	0.000059	0.006873	0.000637	0.955498	0.000000	0.000000
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.962462
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.967268
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.966960
H	71	0.000000	0.000000	0.000000	0.000000	0.000018	0.000000
H	72	0.000000	0.000000	0.000000	0.000000	0.000039	0.000000
H	73	0.000000	0.000000	0.000000	0.000000	0.000041	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.001082	0.000000
H	75	0.000000	0.000000	0.000000	0.000000	0.006911	0.000000
H	76	0.000000	0.000000	0.000000	0.000000	0.006802	0.000000

		C 43	C 44	H 45	H 46	H 47	H 48
C	43	3.867134					
C	44	0.002840	3.861855				
H	45	0.000000	0.000000	0.975878			
H	46	0.000000	0.000000	0.000146	0.976666		
H	47	0.000000	0.000000	0.000165	0.000175	0.971030	
H	48	0.000000	0.000000	0.000169	0.000173	0.000114	0.970145
H	49	0.000000	0.000000	0.000009	0.000007	0.000002	0.000017

H	50	0.000001	0.000000	0.000000	0.000001	0.000000	0.000000
H	51	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000
H	52	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	53	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	54	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	55	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	56	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	58	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	60	0.000026	0.000292	0.000000	0.000000	0.000000	0.000000
H	61	0.000347	0.000276	0.000000	0.000000	0.000000	0.000000
H	62	0.001050	0.000019	0.000000	0.000000	0.000000	0.000000
H	63	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	71	0.961634	0.000019	0.000000	0.000000	0.000000	0.000000
H	72	0.968848	0.000007	0.000000	0.000000	0.000000	0.000000
H	73	0.969691	0.000007	0.000000	0.000000	0.000000	0.000000
H	74	0.000764	0.962439	0.000000	0.000000	0.000000	0.000000
H	75	0.000585	0.966925	0.000000	0.000000	0.000000	0.000000
H	76	0.000542	0.967286	0.000000	0.000000	0.000000	0.000000

		H 49	H 50	H 51	H 52	H 53	H 54
H	49	0.962204					
H	50	0.000003	0.971035				
H	51	0.000343	0.002315	0.975623			
H	52	0.000137	0.000022	0.000247	0.970966		
H	53	0.000006	0.000246	0.000027	0.002379	0.975638	
H	54	0.000007	0.000004	0.000000	0.002256	0.000016	0.968256
H	55	0.000000	0.000000	0.000000	0.000001	0.000000	0.000067
H	56	0.000003	0.000008	0.000001	0.000001	0.000040	0.000142
H	57	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
H	58	0.000000	0.000000	0.000000	0.000002	0.000000	0.000534
H	59	0.000000	0.000000	0.000000	0.000000	0.000000	0.000589
H	60	0.000000	0.000001	0.000043	0.000007	0.000001	0.000000
H	61	0.000000	0.000001	0.000000	0.000000	0.000000	0.000000
H	62	0.000000	0.002559	0.000016	0.000004	0.000000	0.000000
H	63	0.000000	0.000103	0.000005	0.000003	0.000360	0.000000
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000001	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000005	0.000001

H	70	0.000000	0.000000	0.000000	0.000000	0.000005	0.000001
H	71	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000002	0.000000	0.000000	0.000000	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	75	0.000000	0.000000	0.000005	0.000000	0.000000	0.000000
H	76	0.000000	0.000000	0.000005	0.000000	0.000000	0.000000

		H 55	H 56	H 57	H 58	H 59	H 60
H	55	0.969272					
H	56	0.000184	0.973878				
H	57	0.000012	0.000001	0.975714			
H	58	0.000000	0.000000	0.000026	0.980284		
H	59	0.000000	0.000000	0.000033	0.000043	0.979475	
H	60	0.000000	0.000000	0.000000	0.000000	0.000000	0.973908
H	61	0.000000	0.000000	0.000000	0.000000	0.000000	0.000184
H	62	0.000000	0.000000	0.000000	0.000000	0.000000	0.000142
H	63	0.000000	0.000000	0.000000	0.000000	0.000000	0.000003
H	64	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	65	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	66	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	67	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	68	0.000010	0.000013	0.000001	0.000004	0.000003	0.000000
H	69	0.000000	0.000001	0.000003	0.000002	0.000000	0.000000
H	70	0.000000	0.000000	0.000004	0.000000	0.000002	0.000000
H	71	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001
H	72	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	74	0.000000	0.000000	0.000000	0.000000	0.000000	0.000013
H	75	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	76	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001

		H 61	H 62	H 63	H 64	H 65	H 66
H	61	0.969246					
H	62	0.000068	0.968436				
H	63	0.000000	0.000007	0.962071			
H	64	0.000000	0.000000	0.000017	0.970135		
H	65	0.000000	0.000000	0.000009	0.000169	0.975869	
H	66	0.000000	0.000000	0.000007	0.000173	0.000146	0.976664
H	67	0.000000	0.000000	0.000002	0.000114	0.000165	0.000175
H	68	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	69	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	70	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
H	71	0.000012	0.000001	0.000000	0.000000	0.000000	0.000000
H	72	0.000000	0.000590	0.000000	0.000000	0.000000	0.000000
H	73	0.000000	0.000528	0.000000	0.000000	0.000000	0.000000
H	74	0.000010	0.000000	0.000000	0.000000	0.000000	0.000000
H	75	0.000000	0.000001	0.000000	0.000000	0.000000	0.000000

H 76	0.000000	0.000001	0.000000	0.000000	0.000000	0.000000

	H 67	H 68	H 69	H 70	H 71	H 72
H 67	0.971051					
H 68	0.000000	0.977441				
H 69	0.000000	0.000005	0.978338			
H 70	0.000000	0.000003	0.000001	0.978350		
H 71	0.000000	0.000000	0.000000	0.000000	0.975671	
H 72	0.000000	0.000000	0.000000	0.000000	0.000034	0.979444
H 73	0.000000	0.000000	0.000000	0.000000	0.000025	0.000044
H 74	0.000000	0.000000	0.000000	0.000000	0.000001	0.000003
H 75	0.000000	0.000000	0.000000	0.000000	0.000005	0.000002
H 76	0.000000	0.000000	0.000000	0.000000	0.000003	0.000000

	H 73	H 74	H 75	H 76
H 73	0.980357			
H 74	0.000004	0.977422		
H 75	0.000000	0.000002	0.978332	
H 76	0.000002	0.000005	0.000001	0.978347