Supporting information for

Chiral and Prochiral Singlet Radical-Pair Combinations in Reaction Cavities of Polyethylene Films. Control and Analysis of Radical Tumbling and Translation.

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Table S1. Product distributions from irradiations of (*R*)-**2** in unstretched **PE0** films at 23 °C[a]

%Conversionof (*R*)-**2**	**2BN**	**4BN**	**3**	**5**	**6**	**2BN**/**4BN**	(*S*)-**2**/(**2BN** + **4BN**)
3	43.6±0.8	36.3±1.5	17.8±0.8	0.7±0.5	1.6±0.5	1.20±0.05	0.18±0.04
4	42.5±1.0	37.9±1.7	16.5±1.2	1.5±0.5	1.6±0.5	1.12±0.04	0.18±0.04
5	37.7±1.0	35.4±1.4	22.7±2.2	2.9±0.5	1.3±0.5	1.06±0.04	0.21±0.03
6	36.2±0.5	36.9±0.5	24.3±1.2	1.2±0.5	1.4±0.5	0.98±0.04	0.17±0.03
7	30.1±1.2	30.8±1.0	29.7±1.5	7.5±1.0	1.9±0.5	0.98±0.04	0.18±0.03
11	29.3±1.0	30.1±1.1	26.0±1.5	13.1±1.0	1.5±0.5	0.98±0.04	0.16±0.02
13	33.8±1.3	35.5±1.0	21.8±1.0	7.5±1.0	1.4±0.5	0.96±0.04	0.17±0.02
15	34.7±1.0	37.1±1.0	18.9±0.7	7.8±1.0	1.5±0.5	0.93±0.04	0.16±0.02
21	31.5±0.5	38.6±0.5	23.1±1.4	5.2±1.0	1.6±0.5	0.82±0.04	0.15±0.01

[a] Relative yield (%); the sum of relative yields of all products is taken as 100%; the mass balance is > 80%; entries are the average values from at least 3 HPLC analyses on two separate runs with an error of one standard deviation; < 3.5%of **4** was observed when the conversion of (*R*)-**2** was > 13%.

Table S2. *Ee*% of photoproducts from irradiations of (*R*)-**2**[a] in unstretched **PE0** films at 23 °C[b]

% Conversion of (*R*)-**2**	*ee%*		
	remaining **2**	**2BN**	**4BN**
3	99.2	56.4	41.4
4	98.8	55.4	41.2
5	98.4	54.8	40.4
6	98.4	54.8	40.8
7	98.4	53.0	38.8
11	97.8	54.8	39.2
13	96.6	55.6	40.4
15	96.0	55.0	39.7
21	94.6	53.2	37.9

[a] *ee* of (*R*)-**2** before irradiation is 99.5%. [b] ± 1.0%.

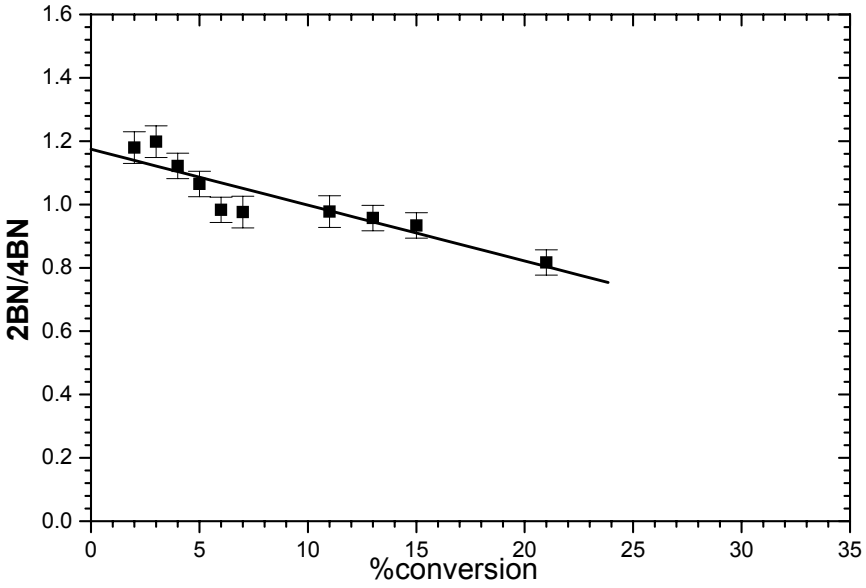

Figure S1. 2BN/4BN ratio *versus* percent of conversion of (*R*)-**2** in unstretched **PE0** films at 23 °C. The straight line is the best fit to data points below *ca*. 20% conversions of (*R*)-**2** and it provides the value extrapolated to 0% conversion.

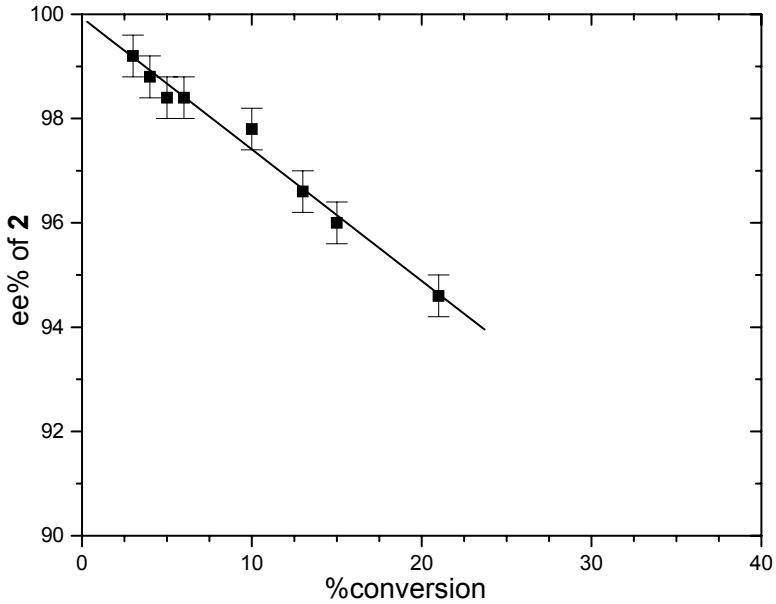

Figure S2. The *ee*% of **2** remaining after irradiation *versus* percent of conversion for irradiations of (*R*)-**2** in unstretched **PE0** films at 23 °C. The straight line is the best fit to data points below *ca*. 20% conversions of (*R*)-**2** and it provides the value extrapolated to 0% conversion.

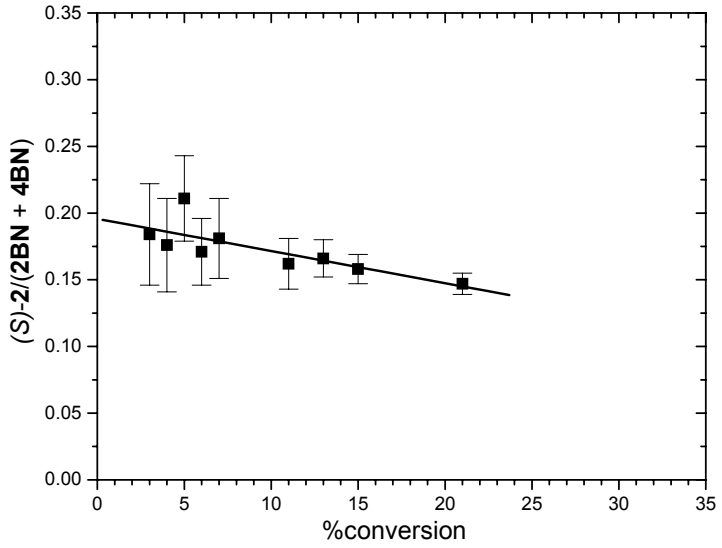

Figure S3. (*S*)-**2**/(**2BN** + **4BN**) *versus* percent of conversion for irradiations of (*R*)-**2** in unstretched **PE0** films at 23 °C. The straight line is the best fit to data points below *ca*. 20% conversions of (*R*)-**2** and it provides the value extrapolated to 0% conversion.

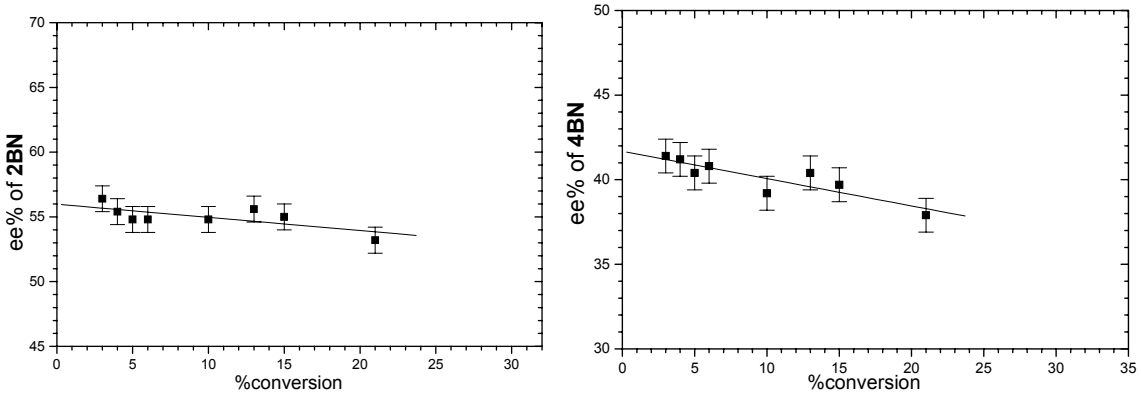

Figure S4. *Ee***%** of **2BN** (left) and **4BN** (right) *versus* percent of conversion for irradiations of (*R*)-**2** in unstretched **PE0** films at 23 °C. The straight line is the best fit to data points below *ca*. 20% conversions of (*R*)-**2** and it provides the value extrapolated to 0% conversion.

Table S3. Product distributions from irradiations of (*R*)-**2** in stretched **PE0** films at 23 °C[a]

%Conversionof (*R*)-**2**	**2BN**	**4BN**	**3**	**5**	**6**	**2BN**/**4BN**	(*S*)-**2**/(**2BN** + **4BN**)
3	39.0±2.8	30.1±1.4	25.7±1.8	4.4±1.0	0.8±0.5	1.29±0.05	0.20±0.05
4	39.5±2.0	31.9±1.5	24.7±1.5	3.2±1.0	0.7±0.5	1.24±0.05	0.17±0.04

7	36.7±1.0	31.3±1.6	25.2±1.5	6.2±1.0	0.6±0.5	1.17±0.05	0.16±0.03
9	39.5±2.0	36.0±1.4	20.4±1.1	3.3±1.0	0.8±0.5	1.10±0.04	0.16±0.02
15	31.8±1.0	35.3±2.4	28.7±1.9	3.4±1.0	0.8±0.5	0.90±0.04	0.16±0.02
16	30.7±1.2	40.4±1.3	25.0±1.1	3.0±1.0	0.9±0.5	0.76±0.04	0.15±0.02

[a] Relative yield (%); the sum of relative yields of all products is taken as 100%; the mass balance is > 80%; entries are the average values from at least 3 HPLC analyses on two separate runs with an error of one standard deviation; the yield of **4** was below our detection limit.

Table S4. *Ee*% of photoproducts from irradiations of (*R*)-**2**[a] in stretched **PE0** films at 23 °C[b]

% Conversion of (*R*)-**2**	*ee%*		
	remaining **2**	**2BN**	**4BN**
3	99.2	57.9	43.3
4	99.0	55.8	40.3
7	98.4	54.6	38.6
9	97.8	54.8	37.4
15	96.0	54.6	36.2
16	96.0	53.6	34.6

[a] *ee* of (*R*)-**2** before irradiation is 99.5%. [b] ± 1.0%.

Table S5. Product distributions from irradiations of (*R*)-**2** in unstretched **PE46** films at 23 °C[a]

%Conversion of (*R*)-**2**	**2BN**	**4BN**	**3**	**5**	**6**	**2BN**/**4BN**	(*S*)-**2**/(**2BN** + **4BN**)
4	37.5±1.1	28.9±1.1	27.1±1.1	5.3±0.5	1.2±0.5	1.30±0.06	0.22±0.04
6	42.5±1.0	33.4±1.0	22.6±1.0	0.5±0.5	1.0±0.5	1.27±0.05	0.19±0.03
9	42.3±2.4	35.7±1.1	18.1±1.0	2.6±0.5	1.3±0.5	1.19±0.08	0.17±0.02
10	42.2±1.0	35.2±1.0	21.1±1.0	0.3±0.5	1.2±0.5	1.20±0.04	0.17±0.02
15	41.5±1.0	35.7±1.0	21.2±1.0	0.2±0.5	1.4±0.5	1.16±0.04	0.17±0.02
21	35.1±1.0	37.9±0.5	23.9±1.0	1.5±0.5	1.6±0.5	0.93±0.03	0.17±0.01
22	32.8±0.7	37.5±1.2	27.1±1.1	1.3±0.5	1.3±0.5	0.88±0.03	0.17±0.01
24	33.0±0.5	43.1±0.5	21.9±2.1	0.2±0.5	1.8±0.5	0.76±0.02	0.17±0.01
29	25.1±0.4	43.5±0.7	24.0±1.0	5.4±0.5	2.0±0.5	0.58±0.02	0.16±0.01

[a] Relative yield (%); the sum of relative yields of all products is taken as 100%; the mass balance is > 80%; entries are the average values from at least 3 HPLC analyses on two separate runs with an error of one standard deviation; < 1.5% of **4** was observed when the conversion of (*R*)-**2** was > 15%.

Table S6. *Ee*% of photoproducts from irradiations of (*R*)-**2**[a] in unstretched **PE46** films at 23 °C[b]

% Conversion of (*R*)-**2**	*ee%*		
	remaining **2**	**2BN**	**4BN**
4	98.6	48.8	31.9
5	98.4	48	32.8
6	98.2	48.8	32.4
9	97.4	47.2	30.6
10	97.0	48.1	32.0
14	95.6	47.4	30.9
15	95.2	46.8	30.4
22	93.6	46.8	29.8
24	92.2	44.3	28.5
29	91.4	43.7	27.8

[a] *ee* of (*R*)-**2** before irradiation is 99.5%. [b] ± 1.0%.

Table S7. Product distributions from irradiations of (*R*)-**2** in stretched **PE46** films at 23 °C[a]

%Conversion of (*R*)-**2**	**2BN**	**4BN**	**3**	**5**	**6**	**2BN/4BN**	(*S*)-**2**/(**2BN** + **4BN**)
5	46.8±2.0	35.5±1.0	13.4±1.0	4.1±0.5	0.2±0.1	1.32±0.07	0.18±0.03
6	46.1±1.1	35.4±1.1	12.8±1.0	5.5±0.5	0.2±0.1	1.30±0.05	0.23±0.03
7	47.0±3.2	38.2±1.6	14.3±1.5	0.3±0.5	0.2±0.1	1.23±0.10	0.23±0.03
9	46.0±0.5	35.2±1.0	14.9±1.0	3.7±0.5	0.2±0.1	1.31±0.04	0.23±0.03
10	46.0±1.0	35.9±1.4	14.0±1.0	3.9±0.5	0.2±0.1	1.28±0.06	0.22±0.02
11	46.0±1.1	38.7±0.9	13.3±0.9	1.9±0.5	0.1±0.1	1.19±0.04	0.18±0.02
19	41.9±1.0	40.0±1.0	15.3±0.5	2.5±0.5	0.3±0.1	1.05±0.04	0.21±0.01
22	41.3±0.5	41.8±1.4	12.6±0.6	4.1±0.5	0.2±0.1	0.99±0.04	0.23±0.01
26	37.9±1.0	45.0±0.5	16.4±0.5	0.3±0.5	0.4±0.2	0.84±0.02	0.20±0.01

[a] Relative yield (%); the sum of relative yields of all products is taken as 100%; the mass balance is > 80%; entries are the average values from at least 3 HPLC analyses on two separate runs with an error of one standard deviation; < 1.5% of **4** was observed when the conversion of (*R*)-**2** was > 11%.

Table S8. *Ee*% of photoproducts from irradiations of (*R*)-**2**[a] in stretched **PE46** films at 23 °C[b]

% Conversion of (*R*)-**2**	*ee%*		
	remaining **2**	**2BN**	**4BN**
5	98.4	41.4	25.2
6	97.2	39.4	23.0
7	97.2	38.7	23.0
9	96.2	37.8	23.0
10	96.2	37.6	23.0
11	96.4	38.2	22.8

19	91.8	34.8	20.1
22	89.6	30.6	19.0
26	88.0	32.0	19.6

[a] *ee* of (*R*)-**2** before irradiation is 99.5%. [b] ± 1.0%.

Table S9. Product Distributions from Irradiations of (*R*)-**1** in **PE** Films (1-7 mmol/kg) and *n*-Hexane (2 mM) at Various Temperatures[a]

Medium[b]	T (°C)	conversion %	**2**	**2BN**	**4BN**	**2AN**	**4AN**	**3**	**4**	**5**
Hexane[c]	23	12-32	3.3±0.1	4.6±0.3	13.3±0.5	46.5±2.7	24.6±2.0	4.9±0.4	0	2.8±0.8
PE0 (u)	- 8	10-15	0.9±0.1	1.3±0.1	6.1±0.5	76.2±1.0	6.5±0.5	4.6±0.1	3.2±0.3	1.2±0.2
	5	19-21	0.9±0.1	1.9±0.1	6.9±0.4	75.0±0.5	7.9±0.4	4.5±0.6	2.2±1.1	0.6±0.1
	23	20-25	1.0±0.1	1.4±0.1	5.6±0.8	70.5±2.5	13.6±0.4	5.2±0.5	2.1±1.2	0.7±0.3
	43	18-21	0.9±0.1	0.9±0.1	6.3±0.5	64.8±1.6	13.4±0.6	7.1±0.8	5.3±0.4	1.4±0.1
	60	20-21	1.1±0.1	1.0±0.1	5.7±0.1	61.3±0.3	15.4±0.3	10.1±1.3	4.2±1.4	1.3±0.1
PE0 (s)	23	26-28	0.8±0.1	1.2±0.1	4.9±0.2	71.3±2.0	12.0±0.2	7.4±2.0	1.9±0.1	0.5±0.2
PE46 (u)	5	24-35	1.3±0.2	1.9±0.2	8.0±1.0	70.3± 2.5	4.7±0.9	3.4±0.3	9.4±3.0	1.0±0.3
	23	29-34	1.1±0.1	0.9±0.1	3.4±0.5	75.8±0.3	7.6±0.3	2.0±0.8	9.0±0.7	0.2±0.1
	43	23-32	1.0±0.1	1.2±0.1	6.0±1.0	63.6±1.3	10.5±1.0	9.6±0.9	6.7±0.3	1.6±0.2
	60	25-33	0.8±0.1	0.8±0.1	2.1±0.3	63.7±0.5	13.0±1.5	11.9±1.1	6.4±0.1	1.5±0.1
PE46 (s)	5	26-30	3.9±0.1	5.4±0.2	28.9±0.2	42.5±0.9	5.2±0.1	5.9±0.1	5.0±1.0	3.3±0.1
	23	27-37	1.5±0.2	1.2±0.1	8.7±0.6	78.1±0.6	5.9±0.1	2.6±0.1	1.6±0.1	0.4±0.1
	43	25-28	1.0±0.1	1.4±0.1	8.1±0.4	58.1±2.1	9.0±1.2	8.0±0.7	11.6±0.8	2.8±0.6
PE74 (u)	5	23	1.9±0.3	2.7±0.4	8.8±1.2	65.8±2.5	7.4±1.2	3.8±1.2	8.8±1.5	0.8±0.1
	23	26	0.9±0.1	1.6±0.2	4.2±0.2	80.1±2.3	9.1±1.0	2.1±0.3	2.0±0.1	0
PE74 (s)	5	17	5.6±0.5	6.5±0.5	29.0±3.5	39.9±3.0	6.7±0.5	5.6±1.0	3.4±0.3	3.3±0.3
	23	20	2.2±0.5	4.5±0.5	13.9±2.0	52.5±3.0	11.6±1.0	3.8±0.5	9.1±1.5	2.4±0.5

[a] Relative yield (%); the sum of relative yields of all products is taken as 100%. The mass balance is > 80% and conversions of **1** were < 35%. Each entry is the average of at least 2 experiments and 3 HPLC analyses with an error of one standard deviation. [b] 'u' and 's' refer to unstretched and stretched films, respectively. [c] Small amounts of a decarboxylated product, 1-(1-naphthyl)-1-phenylethane (< 2%), and a cage-escape product **6** (*ca*. 7%) are not reported.

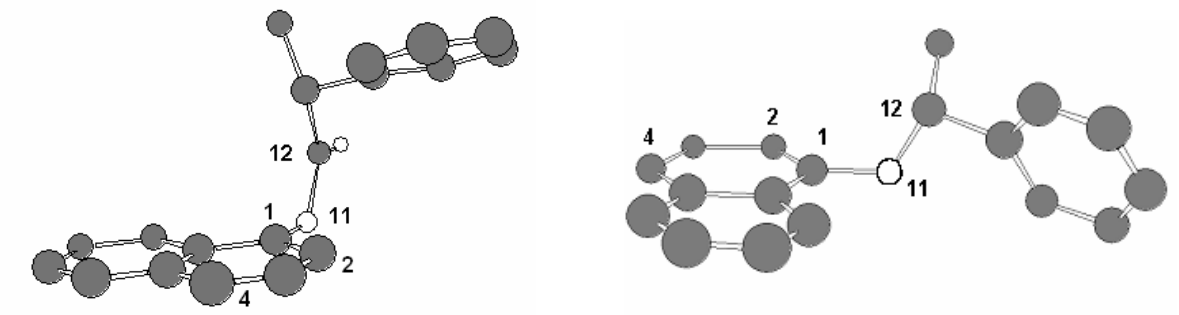

Figure S5. Calculated optimized geometries of **1-L** (left) and **2-L** (right) in their ground states. The solid and open circles represent carbon and oxygen atoms, respectively; hydrogen atoms have not been included for clarity.

Table S10. Cartesian coordinates of optimized **1-G** in its ground state calculated at the RHF/6-31G* level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.159488	1.461056	-0.258454
2	6	0	-1.681463	2.697842	-0.050605
3	6	0	-3.062431	2.860370	0.215931
4	6	0	-3.881193	1.778371	0.264386
5	6	0	-3.371050	0.469886	0.052403
6	6	0	-1.994363	0.312876	-0.207905
7	6	0	-1.505688	-1.004033	-0.415609
8	6	0	-2.318828	-2.084913	-0.380166
9	6	0	-3.697675	-1.914211	-0.115648
10	6	0	-4.209552	-0.675129	0.095335
11	8	0	-0.166443	-1.145522	-0.728023
12	6	0	0.688580	-1.656562	0.169043
13	6	0	2.108485	-1.627341	-0.367224
14	6	0	2.961105	-2.718767	0.287277
15	6	0	2.696425	-0.232662	-0.174269
16	6	0	3.196322	0.475610	-1.258946
17	6	0	3.758356	1.731700	-1.087667
18	6	0	3.822252	2.297766	0.173666
19	6	0	3.320291	1.601130	1.262239
20	6	0	2.762642	0.345948	1.090449
21	8	0	0.367853	-2.057058	1.235505
22	1	0	-0.114050	1.341570	-0.466519
23	1	0	-1.044050	3.562847	-0.089026
24	1	0	-3.458561	3.846822	0.378200
25	1	0	-4.931457	1.897420	0.464766
26	1	0	-1.913410	-3.065480	-0.543982
27	1	0	-4.334230	-2.779633	-0.083598
28	1	0	-5.258040	-0.544643	0.296413
29	1	0	2.042257	-1.814287	-1.432026
30	1	0	3.966270	-2.689750	-0.117600
31	1	0	3.016893	-2.582493	1.358974

32	1	0	2.542259	-3.701238	0.097507
33	1	0	3.148082	0.046088	-2.244211
34	1	0	4.142441	2.264543	-1.939219
35	1	0	4.256522	3.272204	0.308503
36	1	0	3.361320	2.034940	2.245351
37	1	0	2.370109	-0.181892	1.941195

Calculations of optimized **1-G** in its ground state calculated at the RHF/6-31G* level also provide:

(1) SCF Done: E (RHF) = -878.577303668 A.U.

(2) Zero-point correction = 0.321376 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

Calculations of optimized **1-G** in its ground state calculated at the B3LYP/6-31G* level provide:

(1) SCF Done: E(RB+HF-LYP) = -884.132267205 A.U.

(2) Zero-point correction = 0.299866 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

Table S11. Cartesian coordinates of optimized **1-L** in its ground state calculated at the RHF/6-31G* level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.742877	-1.296400	-0.112734
2	6	0	3.939130	-1.410913	0.522161
3	6	0	4.638014	-0.257241	0.950252
4	6	0	4.122802	0.978851	0.722347
5	6	0	2.876847	1.136777	0.060463
6	6	0	2.177407	-0.015751	-0.351492
7	6	0	0.922413	0.161321	-0.998351
8	6	0	0.419730	1.392050	-1.255195
9	6	0	1.136560	2.542063	-0.845048
10	6	0	2.324506	2.419809	-0.200837
11	8	0	0.256803	-0.957162	-1.441671
12	6	0	-0.640542	-1.654487	-0.720118
13	6	0	-1.090113	-1.111941	0.631772
14	6	0	-1.406567	-2.279563	1.576391
15	6	0	-2.292770	-0.185567	0.461495
16	6	0	-2.325647	1.034278	1.126687
17	6	0	-3.429692	1.865654	1.030080
18	6	0	-4.517365	1.489229	0.259954
19	6	0	-4.493017	0.276316	-0.409016
20	6	0	-3.390879	-0.556901	-0.307952
21	8	0	-1.061333	-2.658744	-1.182729
22	1	0	2.225922	-2.172368	-0.455959
23	1	0	4.364604	-2.382742	0.696109
24	1	0	5.582982	-0.365770	1.451454

25	1	0	4.655170	1.858158	1.039499
26	1	0	-0.521072	1.485221	-1.763623
27	1	0	0.724928	3.513492	-1.049751
28	1	0	2.867611	3.293197	0.113662
29	1	0	-0.284971	-0.532714	1.061724
30	1	0	-1.716647	-1.891086	2.539715
31	1	0	-2.200367	-2.896625	1.178763
32	1	0	-0.532819	-2.905658	1.723741
33	1	0	-1.482741	1.339352	1.721782
34	1	0	-3.437360	2.805194	1.553501
35	1	0	-5.374346	2.133992	0.181172
36	1	0	-5.332264	-0.024416	-1.010421
37	1	0	-3.384536	-1.495488	-0.831317

Calculations of optimized **1-L** in its ground state calculated at the RHF/6-31G* level also provide:

(1) SCF Done: E(RHF) = -878.567723837 A.U.

(2) Zero-point correction = 0.321495 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

Calculations of optimized **1-L** in its ground state calculated at the B3LYP/6-31G* level provide:

(1) SCF Done: E(RB+HF-LYP) = -884.124918119 A.U.

(2) Zero-point correction = 0.299707 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

Table S12. Cartesian coordinates of optimized **1-G** in its first excited singlet state calculated at the CIS/6-31G* level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.196896	1.473747	-0.293159
2	6	0	-1.767003	2.727683	-0.096614
3	6	0	-3.143350	2.857964	0.181814
4	6	0	-3.951308	1.728882	0.259894
5	6	0	-3.431570	0.440044	0.068409
6	6	0	-1.973554	0.308130	-0.216549
7	6	0	-1.472288	-0.988666	-0.396341
8	6	0	-2.273613	-2.118794	-0.333374
9	6	0	-3.649371	-1.981483	-0.062816
10	6	0	-4.210298	-0.724858	0.133277
11	8	0	-0.139226	-1.112742	-0.724122
12	6	0	0.727374	-1.669624	0.134639
13	6	0	2.141234	-1.600246	-0.413024
14	6	0	3.017183	-2.699972	0.194630
15	6	0	2.708855	-0.203675	-0.177779
16	6	0	3.188523	0.548869	-1.241517
17	6	0	3.732055	1.807261	-1.031760
18	6	0	3.797326	2.331129	0.247615
19	6	0	3.315320	1.590015	1.315606

20	6	0	2.776190	0.332635	1.105273
21	8	0	0.418140	-2.132263	1.179044
22	1	0	-0.149123	1.393846	-0.507782
23	1	0	-1.149784	3.604486	-0.157301
24	1	0	-3.568695	3.832389	0.333050
25	1	0	-5.000231	1.836761	0.471363
26	1	0	-1.836970	-3.086953	-0.479712
27	1	0	-4.265431	-2.858949	-0.007787
28	1	0	-5.261967	-0.636878	0.338867
29	1	0	2.066770	-1.751336	-1.483113
30	1	0	4.017206	-2.641645	-0.219655
31	1	0	3.083136	-2.599356	1.269718
32	1	0	2.610939	-3.681647	-0.023863
33	1	0	3.139077	0.152330	-2.240440
34	1	0	4.100910	2.374729	-1.867526
35	1	0	4.217296	3.307242	0.412235
36	1	0	3.357456	1.990856	2.312557
37	1	0	2.399244	-0.230071	1.940674

Calculations of optimized **1-G** in its first excited singlet state calculated at the CIS/6-31G* level also provide:

(1) SCF Done: E(RHF) = -878.569502367 A.U.

(2) Zero-point correction = 0.318721 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

(4) Excited state 1: Singlet-?Sym 5.1744 eV 239.61 nm f=0.0013

$72 \rightarrow 74$ -0.48138

$73 \rightarrow 75$ 0.50239

This state for optimization and/or second-order correction.

Table S13. Cartesian coordinates of optimized **1-L** in its first excited singlet state calculated at the CIS/6-31G* level.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.738835	-1.304971	-0.141307
2	6	0	3.958281	-1.420636	0.517786
3	6	0	4.643520	-0.272848	0.967850
4	6	0	4.115177	0.993214	0.741571
5	6	0	2.893644	1.170060	0.074275
6	6	0	2.156473	-0.048102	-0.367673
7	6	0	0.918364	0.145312	-1.000043
8	6	0	0.406377	1.407305	-1.269753
9	6	0	1.121347	2.552130	-0.865036
10	6	0	2.337098	2.427862	-0.201516
11	8	0	0.234457	-0.953079	-1.451270
12	6	0	-0.650090	-1.662094	-0.721185

13	6	0	-1.090889	-1.119886	0.633197
14	6	0	-1.408464	-2.286219	1.578314
15	6	0	-2.288764	-0.187085	0.466689
16	6	0	-2.307752	1.038655	1.121467
17	6	0	-3.407510	1.876068	1.027563
18	6	0	-4.504174	1.500027	0.270324
19	6	0	-4.493512	0.281311	-0.388606
20	6	0	-3.395988	-0.557973	-0.289889
21	8	0	-1.068637	-2.666883	-1.183141
22	1	0	2.242295	-2.187192	-0.498109
23	1	0	4.382843	-2.393402	0.680630
24	1	0	5.581970	-0.377397	1.479103
25	1	0	4.652116	1.862644	1.076641
26	1	0	-0.531298	1.491973	-1.782925
27	1	0	0.718891	3.525515	-1.072011
28	1	0	2.869949	3.310307	0.104121
29	1	0	-0.279255	-0.545803	1.057831
30	1	0	-1.711347	-1.897194	2.543647
31	1	0	-2.207569	-2.899233	1.184813
32	1	0	-0.536914	-2.916547	1.720085
33	1	0	-1.457837	1.343556	1.706448
34	1	0	-3.404609	2.820037	1.542901
35	1	0	-5.357764	2.149501	0.193648
36	1	0	-5.339919	-0.019003	-0.980062
37	1	0	-3.399944	-1.500839	-0.805623

Calculations of optimized **1-L** in its first excited singlet state calculated at the CIS/6-31G* level provide:

(1) SCF Done: E(RHF) = -878.559929026 A.U.

(2) Zero-point correction = 0.318729 (Hartree/Particle)

(3) Number of imaginary frequencies: 0

(4) Excited State 1: Singlet-?Sym 5.1548 eV 240.52 nm f=0.0019

$71 \rightarrow 74$ -0.12316

$72 \rightarrow 74$ -0.45380

$73 \rightarrow 75$ 0.49603

This state for optimization and/or second-order correction.