Supporting Information for

Theoretical Calculation of Electronic Circular Dichroism on a Hexahydroxydiphenyl-containing Flavanone Glycoside

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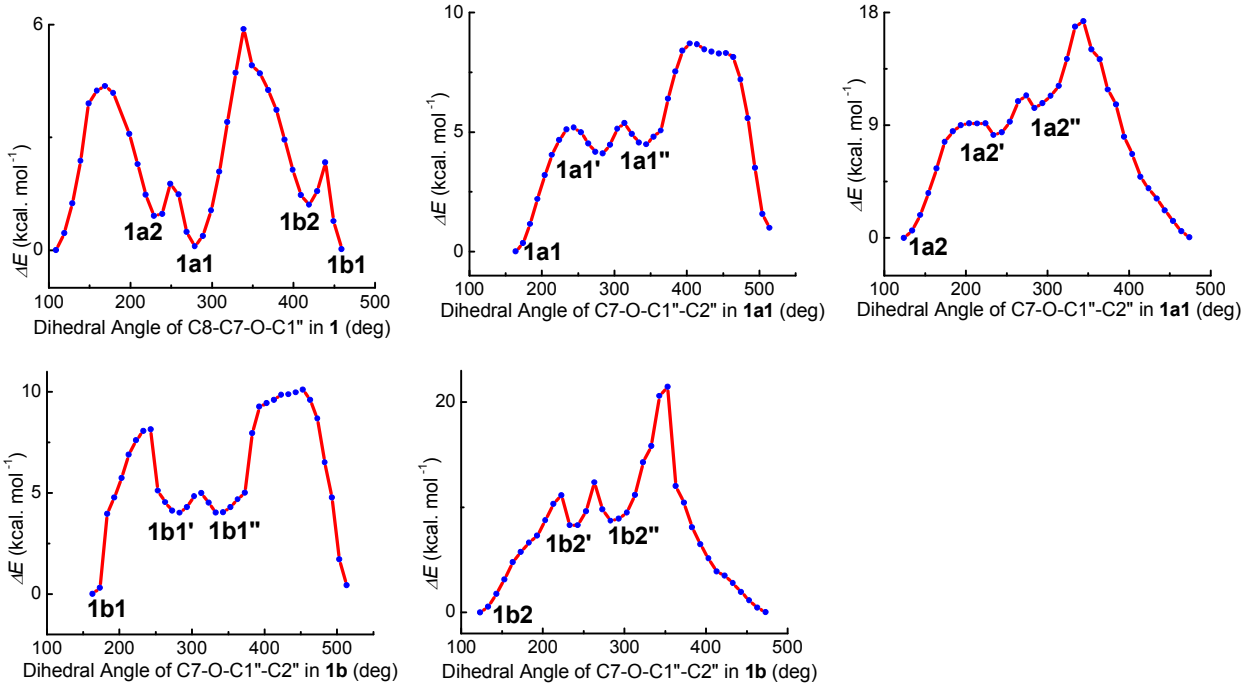

Figure S1. Potential energy surfaces of **1** at the B3LYP/6-31G** level in the gas phase.

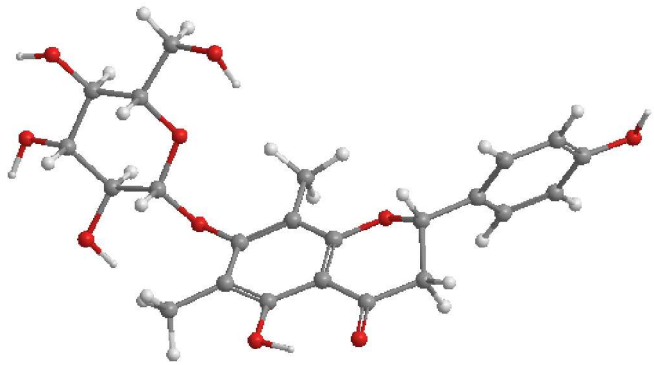

Figure S2. Optimized geometry of conformer of mattucinol-7-*O*-β-L-glucopyranoside (L-**1a1**) at the B3LYP/6-31G** level in the gas phase.

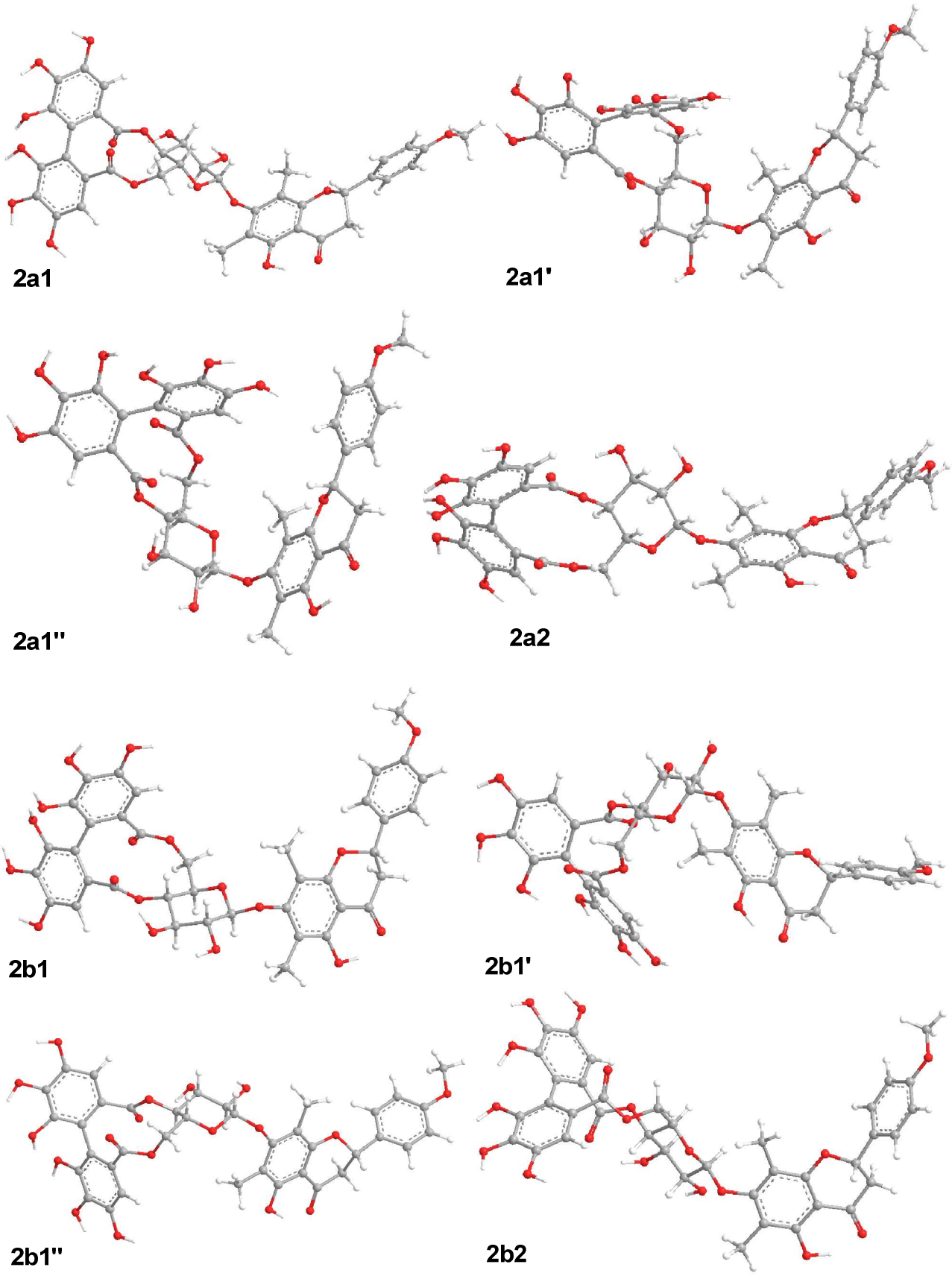

Figure S3. Optimized geometries of compound **2** at the B3LYP/6-31G** level in the gas phase.

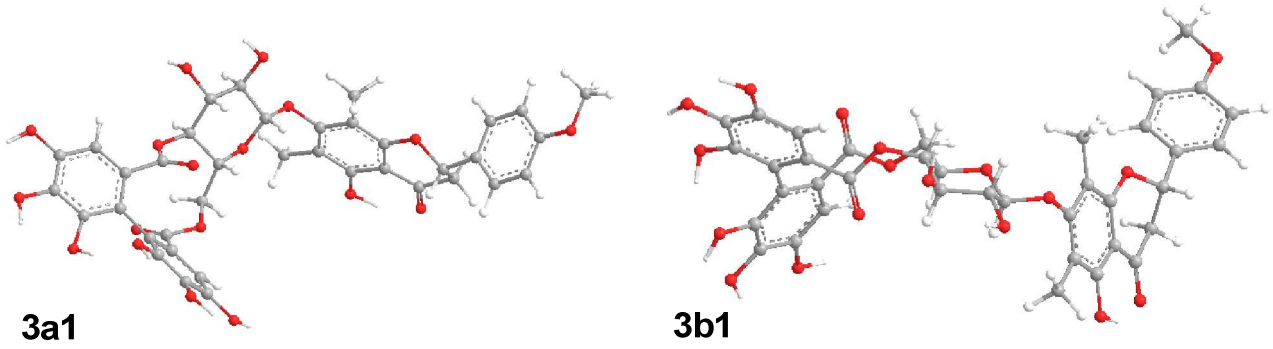

Figure S4. Optimized geometries of compound **3** at the B3LYP/6-31G** level in the gas phase.

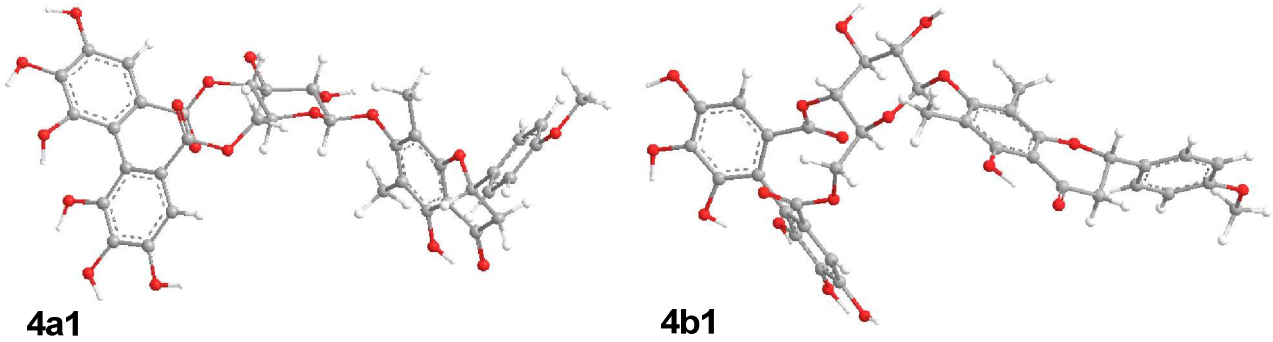

Figure S5. Optimized geometries of compound **4** at the B3LYP/6-31G** level in the gas phase.

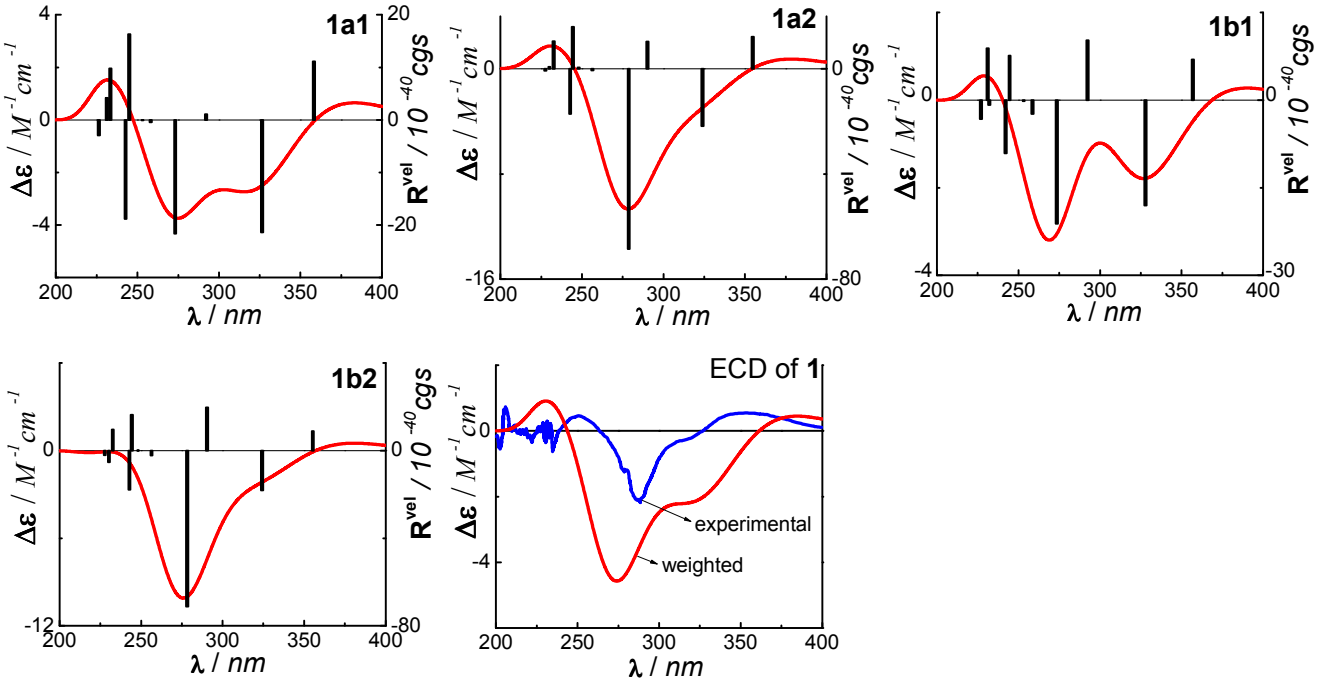

Figure S6. Experimental and calculated ECD of **1** at the B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model in MeOH (σ = 0.20eV).

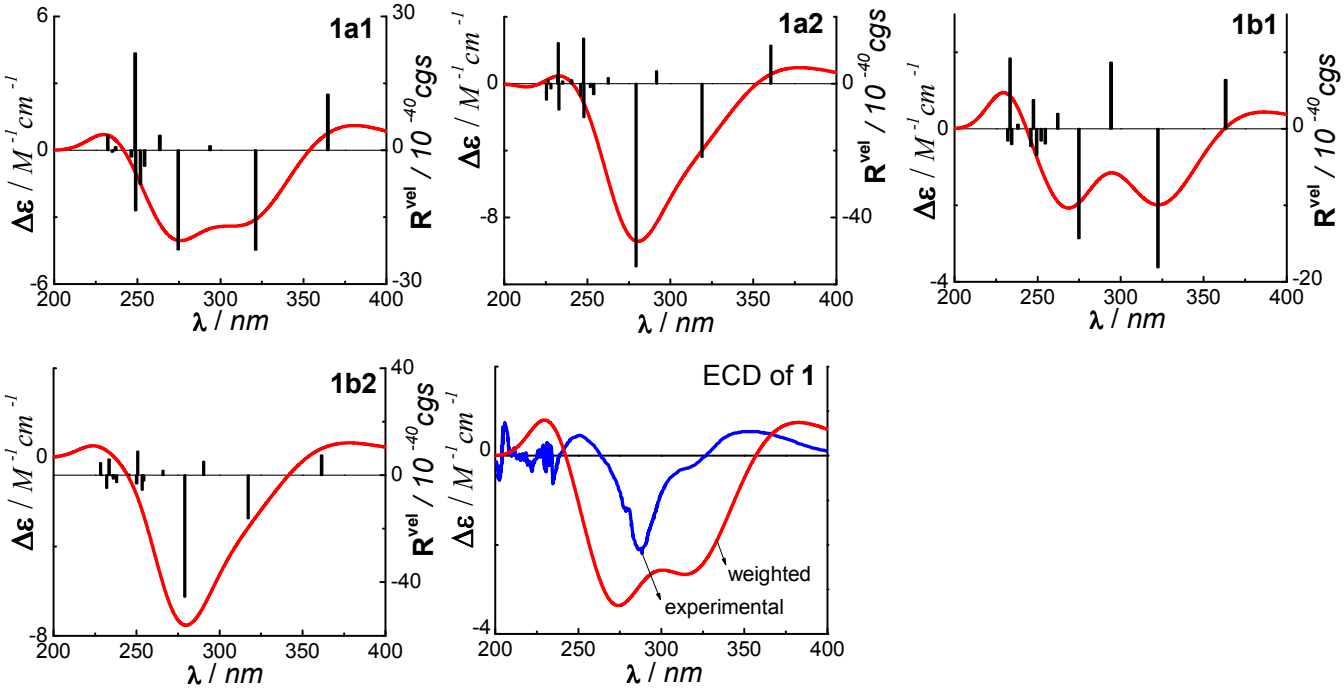

Figure S7. Experimental and calculated ECD of **1** at the B3LYP/6-311++G**//B3LYP/6-31G** level in the gas phase (σ = 0.20eV).

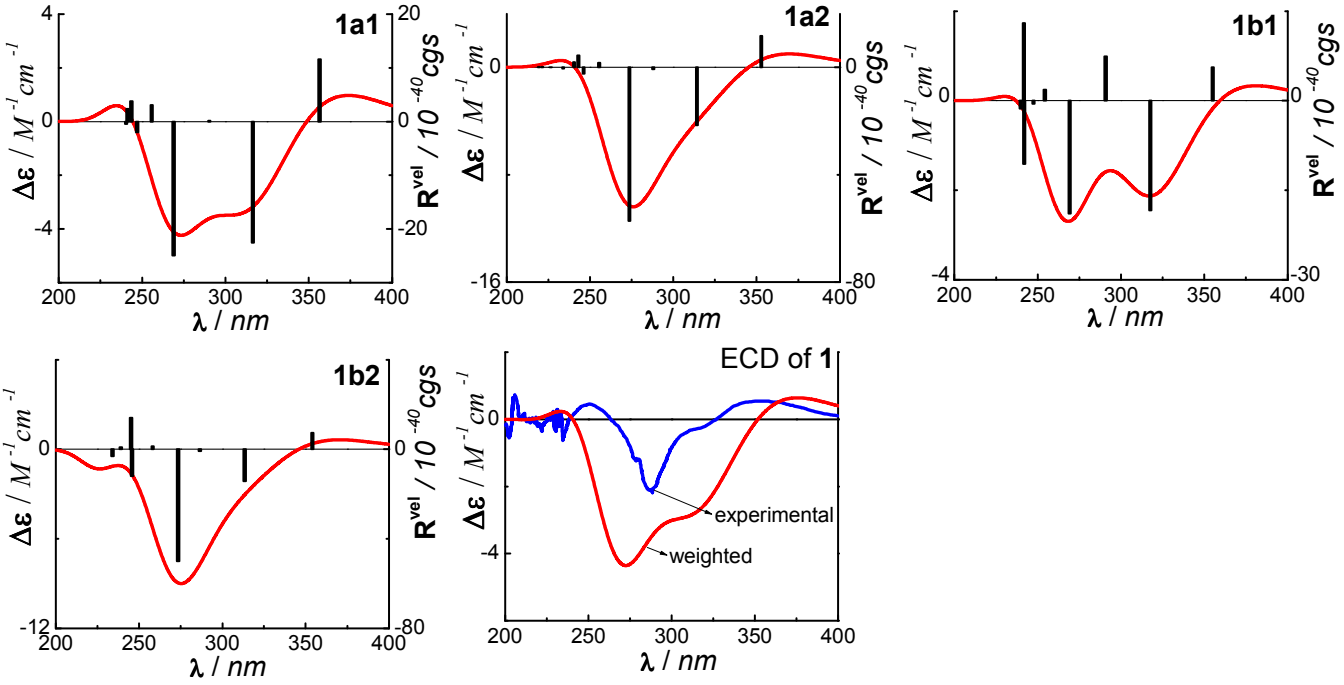

Figure S8. Experimental and calculated ECD of **1** at the B3PW91/6-31G**//B3LYP/6-31G** level in the gas phase (σ = 0.20eV).

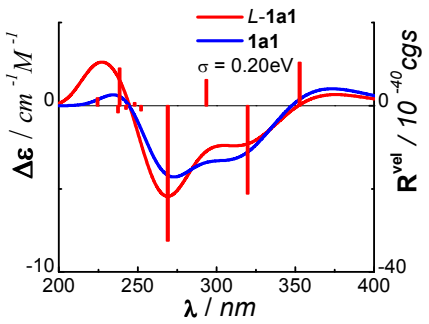

Figure S9. Calculated ECD of L-**1a1** and **1a1** at the B3LYP/6-31G** level in the gas phase.

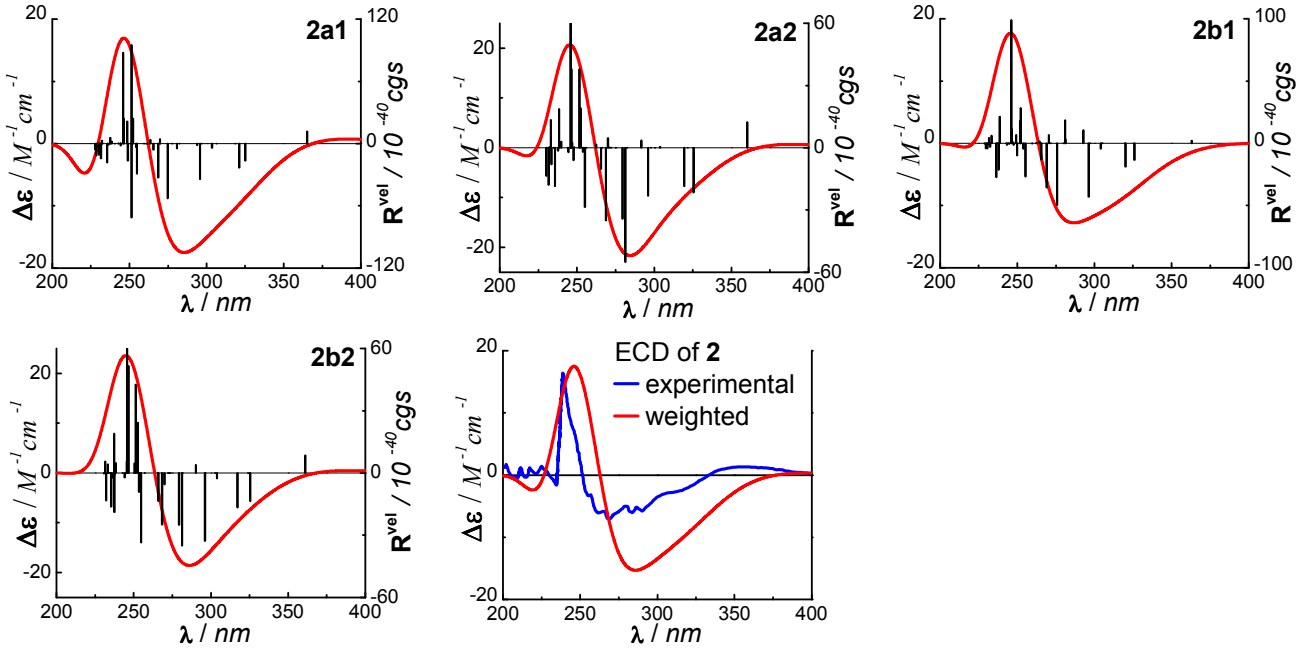

Figure S10. Experimental and calculated ECD of **2** at the B3LYP/6-311++G**//B3LYP/6-31G** level in the gas phase (σ = 0.20eV).

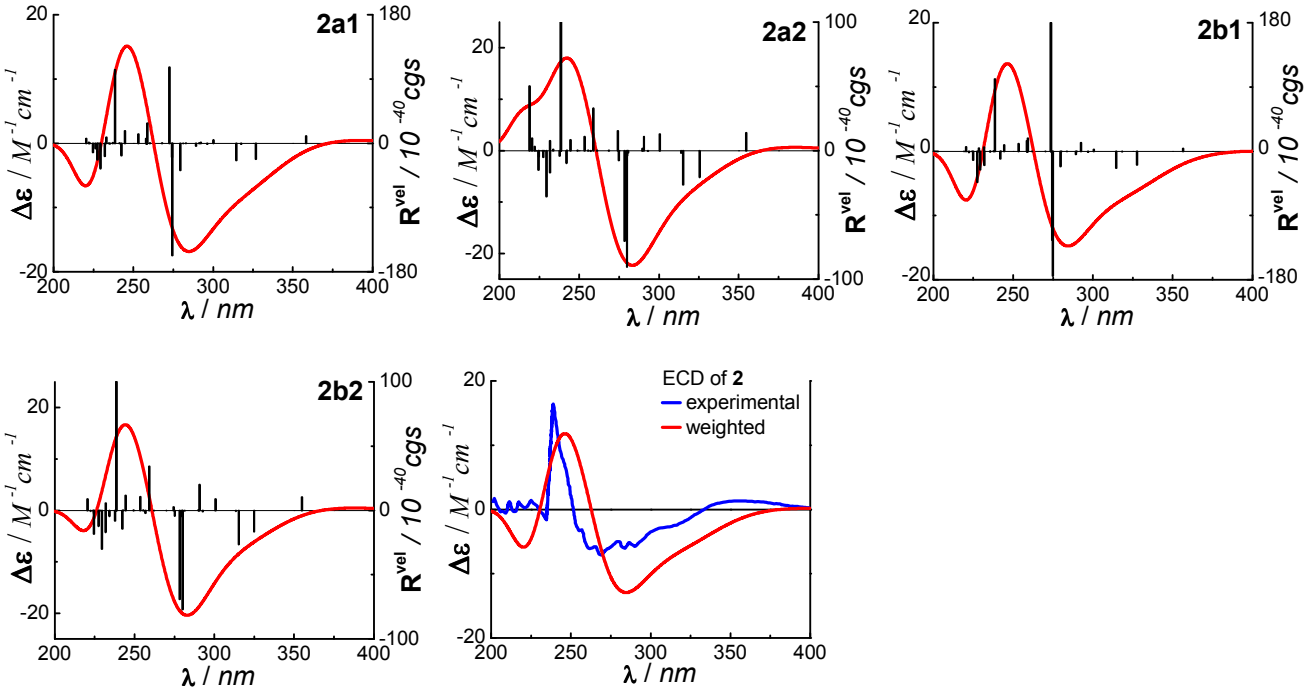

Figure S11. Experimental and calculated ECD of **2** at the B3LYP-SCRF/6-31G**//B3LYP/ 6-31G** level with COSMO model in MeOH (σ = 0.20eV).

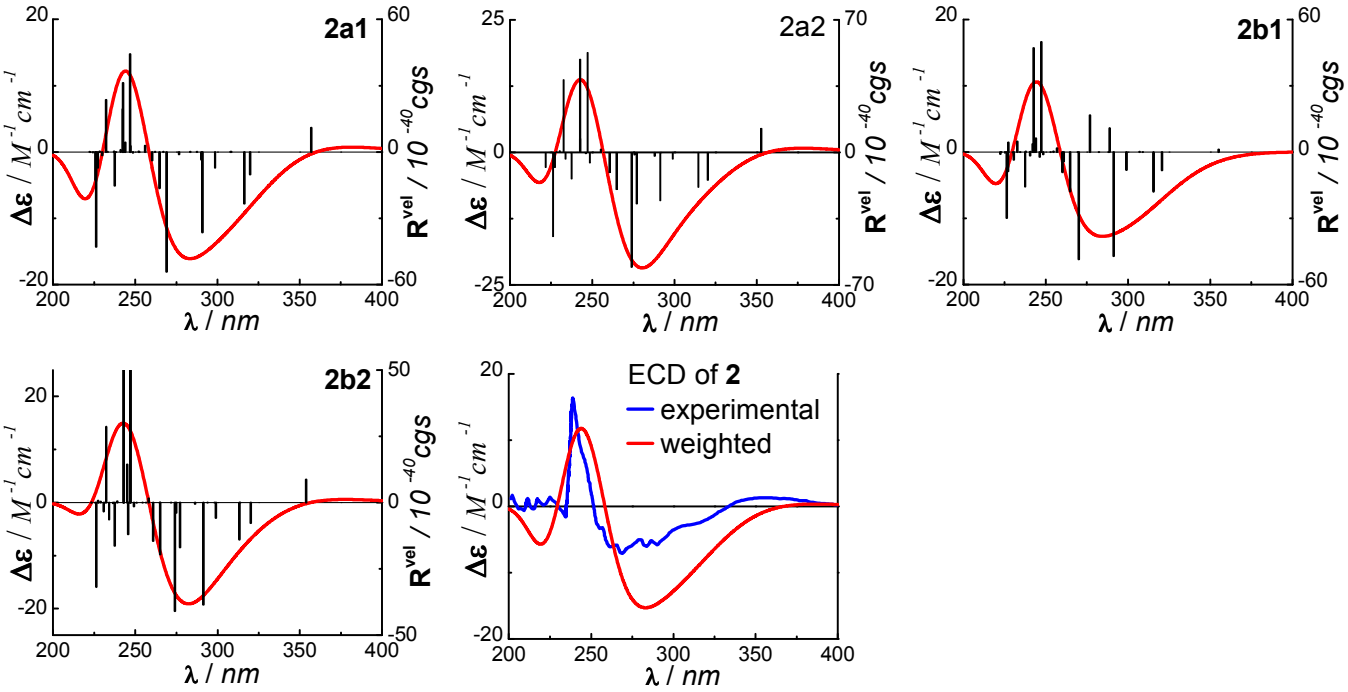

Figure S12. Experimental and calculated ECD of **2** at the B3PW91/6-31G**//B3LYP/6-31G** level in the gas phase (σ = 0.20eV).

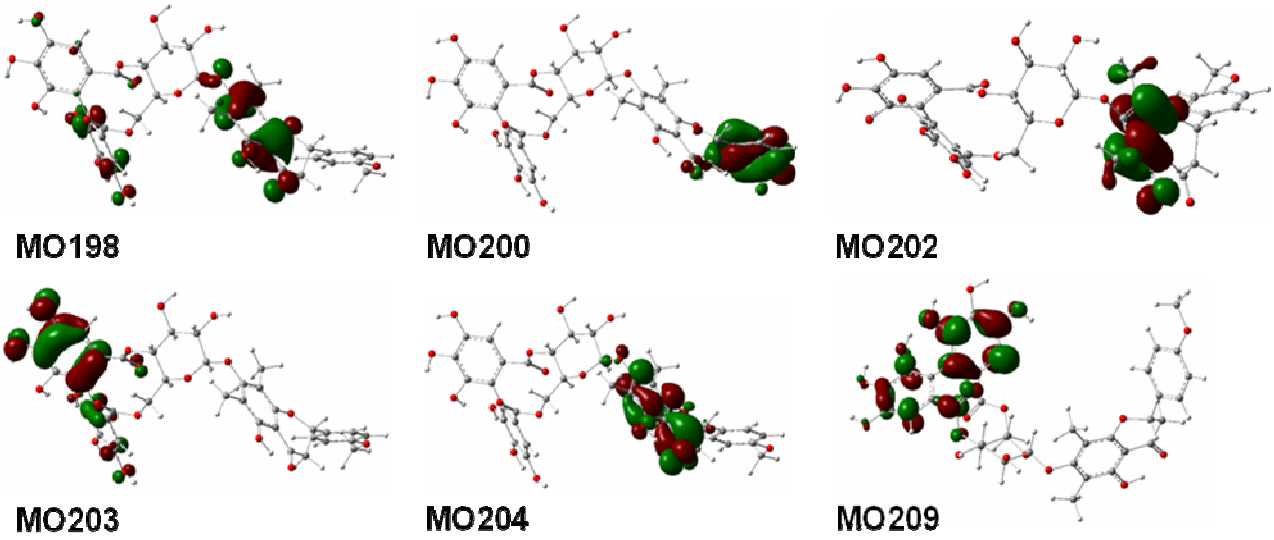

Figure S13. Molecular orbitals involved in key transitions in ECD spectrum of **4b1** at the B3LYP/6-31G** level in the gas phase.

Table S1. Optimized Z-Matrixes of **1** in the Gas Phase (Å).

1a1				**1a1′**			
O	-2.266630	0.117788	-0.244365	O	1.905254	0.393543	0.398097
C	-3.254209	0.790310	0.567736	C	2.789109	0.687960	-0.705950
C	-3.481439	2.211438	0.041148	C	2.948866	2.204885	-0.853264
C	-2.174962	2.974403	-0.049745	C	1.600279	2.885436	-0.980945
C	0.262326	2.807576	-0.548148	C	-0.783653	2.851431	-0.252317
C	1.393503	2.057523	-0.901804	C	-1.839974	2.282433	0.478769
C	1.233448	0.668901	-1.004222	C	-1.589714	1.061075	1.123957
C	0.012501	-0.010135	-0.806251	C	-0.325715	0.425102	1.139746
C	-1.083985	0.772423	-0.442508	C	0.689937	1.020186	0.393092
C	-0.990504	2.178960	-0.311576	C	0.490667	2.228859	-0.316194
C	-4.507202	-0.051366	0.579377	C	4.094300	-0.032355	-0.469161
C	-4.992435	-0.644929	-0.588137	C	4.689970	-0.055359	0.793984
C	-6.177492	-1.382595	-0.587225	C	5.920552	-0.680229	1.003349
C	-6.903867	-1.525697	0.601683	C	6.580575	-1.288849	-0.071555
C	-6.425866	-0.934414	1.779807	C	5.991623	-1.272253	-1.343870
C	-5.239628	-0.212563	1.763362	C	4.761888	-0.655238	-1.532489
O	2.340417	-0.076929	-1.391732	O	-2.599580	0.491623	1.892793
C	3.032000	-0.762202	-0.387171	C	-3.439578	-0.502507	1.346380
C	3.925509	-1.810946	-1.052031	C	-4.563609	0.043098	0.453581
C	4.856927	-2.429116	-0.010412	C	-5.337928	-1.112820	-0.178746
C	5.627009	-1.357495	0.748132	C	-4.404552	-2.067938	-0.906399

C	4.625775	-0.372514	1.371285	C	-3.336762	-2.558364	0.081770
O	3.827189	0.186797	0.320860	O	-2.644182	-1.422964	0.616950
O	-2.150946	4.211831	0.057760	O	1.484656	3.962318	-1.589514
O	0.387742	4.140018	-0.445955	O	-1.004126	4.018782	-0.876339
C	2.697715	2.761814	-1.168610	C	-3.136651	3.044037	0.579384
C	-0.142529	-1.500041	-0.992244	C	-0.030974	-0.808028	1.956988
O	-8.072393	-2.219226	0.719318	O	7.784840	-1.923382	0.015145
C	-8.606355	-2.840318	-0.440164	C	8.428423	-1.976243	1.279323
O	3.106840	-2.804039	-1.639990	O	-5.427143	0.823742	1.260241
O	5.716123	-3.323938	-0.702298	O	-6.304541	-0.536263	-1.045203
O	6.412464	-2.031204	1.733167	O	-5.208767	-3.137806	-1.405767
C	5.286841	0.808565	2.072799	C	-2.261161	-3.426655	-0.562616
O	6.155731	1.522566	1.209065	O	-1.604758	-2.753264	-1.623352
H	-2.851455	0.856970	1.589567	H	2.318522	0.296647	-1.620462
H	-4.179039	2.760893	0.678410	H	3.564946	2.454204	-1.721050
H	-3.923148	2.162856	-0.963347	H	3.455589	2.607029	0.034374
H	-0.514114	4.492954	-0.224339	H	-0.145229	4.278381	-1.303059
H	3.406381	2.089425	-1.650300	H	-3.832377	2.566466	1.266659
H	2.533984	3.635973	-1.805202	H	-2.938618	4.065819	0.919301
H	3.145978	3.127899	-0.237354	H	-3.619966	3.138146	-0.400344
H	-0.264307	-2.017032	-0.032477	H	0.093306	-1.695990	1.328378
H	-1.041828	-1.717330	-1.575542	H	0.902032	-0.678933	2.513266
H	0.719077	-1.927397	-1.505231	H	-0.838718	-1.002892	2.660976
H	-4.427653	-0.548212	-1.510000	H	4.177833	0.403644	1.633722
H	-6.519444	-1.838118	-1.508716	H	6.349353	-0.688174	1.998178
H	-9.531835	-3.322869	-0.123264	H	9.362177	-2.516721	1.118803
H	-8.832437	-2.107119	-1.224702	H	8.653965	-0.972534	1.661371
H	-7.924213	-3.599179	-0.844011	H	7.823173	-2.514294	2.019924
H	-6.995971	-1.063418	2.693629	H	6.511899	-1.756805	-2.163150
H	-4.876036	0.231383	2.686902	H	4.312606	-0.659627	-2.522568
H	2.332721	-1.244791	0.313989	H	-3.891201	-0.988066	2.223694
H	4.533233	-1.292594	-1.809670	H	-4.114095	0.639392	-0.354026
H	3.701516	-3.523534	-1.897669	H	-6.190334	1.038979	0.704063
H	4.239261	-2.984067	0.716445	H	-5.840164	-1.674400	0.627623
H	6.334556	-3.667354	-0.041317	H	-6.755043	-1.276616	-1.476784
H	6.267066	-0.804538	0.050267	H	-3.903428	-1.540077	-1.726697
H	7.175178	-1.475162	1.936558	H	-4.767042	-3.507421	-2.180606
H	3.991798	-0.911525	2.095017	H	-3.826255	-3.126515	0.889713
H	4.501788	1.456616	2.488108	H	-1.554329	-3.749118	0.215488
H	5.893683	0.441584	2.906643	H	-2.723965	-4.323697	-0.986314
H	5.614474	1.812858	0.460471	H	-1.253375	-1.933442	-1.245783
1a1″				**1a2**			
O	-1.798393	0.401373	-0.313733	O	2.446666	0.118189	0.201852
C	-2.827605	0.863732	0.587669	C	3.487691	0.685061	-0.622477
C	-3.203708	2.308138	0.244454	C	3.638383	2.175883	-0.304360

C	-1.979332	3.201805	0.240401	C	2.313011	2.896920	-0.450079
C	0.455843	3.344730	-0.285580	C	-0.158607	2.715635	-0.209796
C	1.647119	2.756424	-0.734145	C	-1.313816	1.996484	0.139488
C	1.626029	1.378802	-0.998108	C	-1.141699	0.640174	0.457663
C	0.475260	0.567208	-0.899182	C	0.108052	-0.017905	0.492119
C	-0.685131	1.187120	-0.430645	C	1.229216	0.739556	0.163188
C	-0.725782	2.567531	-0.121708	C	1.124885	2.106907	-0.197899
C	-3.989724	-0.096277	0.506721	C	4.750961	-0.109220	-0.394784
C	-4.438180	-0.589490	-0.720633	C	5.138213	-0.500653	0.888856
C	-5.541201	-1.441300	-0.799852	C	6.329494	-1.195079	1.105932
C	-6.222392	-1.803942	0.368877	C	7.161466	-1.500305	0.021509
C	-5.781369	-1.314309	1.606560	C	6.782316	-1.113199	-1.271651
C	-4.675827	-0.476207	1.668341	C	5.588931	-0.431420	-1.471041
O	2.807696	0.849446	-1.500465	O	-2.208238	-0.154954	0.837466
C	3.676999	0.034101	-0.754269	C	-3.331144	-0.289318	0.004262
C	3.536344	0.106965	0.772446	C	-3.504606	-1.759717	-0.392599
C	4.465044	-0.922000	1.418612	C	-4.845986	-1.955811	-1.094029
C	4.241009	-2.316744	0.857052	C	-5.987250	-1.432559	-0.235106
C	4.403677	-2.262032	-0.669075	C	-5.715459	0.039955	0.110263
O	3.471513	-1.309083	-1.191807	O	-4.448005	0.134182	0.776617
O	-2.078623	4.413361	0.497731	O	2.276559	4.105915	-0.739991
O	0.439202	4.660544	-0.020438	O	-0.289284	4.014555	-0.521395
C	2.889419	3.582862	-0.939802	C	-2.628588	2.732566	0.217257
C	0.444788	-0.882975	-1.313974	C	0.206361	-1.480138	0.847213
O	-7.311260	-2.624388	0.410601	O	8.346813	-2.169232	0.116011
C	-7.799343	-3.157765	-0.811074	C	8.782417	-2.587501	1.400608
O	3.884413	1.406652	1.210098	O	-2.437873	-2.121266	-1.251089
O	4.229092	-0.860233	2.818406	O	-4.972178	-3.342881	-1.373003
O	5.201321	-3.172160	1.479195	O	-7.187378	-1.597210	-0.992107
C	4.095296	-3.584190	-1.362177	C	-6.735922	0.634509	1.074654
O	2.801074	-4.069217	-1.042739	O	-6.819212	-0.106237	2.280665
H	-2.409705	0.844078	1.605395	H	3.176437	0.580642	-1.672602
H	-3.938533	2.703721	0.950301	H	4.379951	2.647329	-0.954480
H	-3.658334	2.340008	-0.754887	H	3.986182	2.294885	0.730581
H	-0.491243	4.885320	0.245620	H	0.630688	4.358996	-0.683009
H	3.632371	3.356602	-0.169751	H	-3.331370	2.222851	0.876386
H	3.343803	3.360835	-1.909698	H	-2.457290	3.745020	0.590519
H	2.647475	4.644995	-0.895529	H	-3.100633	2.841688	-0.767716
H	0.651370	-1.557670	-0.473399	H	1.230994	-1.830899	0.723782
H	-0.543833	-1.142774	-1.696978	H	-0.095214	-1.656629	1.885756
H	1.194638	-1.070064	-2.082932	H	-0.456832	-2.070946	0.209925
H	-3.907958	-0.321669	-1.629075	H	4.491298	-0.278890	1.731687
H	-5.856102	-1.813278	-1.767355	H	6.594833	-1.491927	2.113453
H	-8.659339	-3.774727	-0.547345	H	9.737744	-3.090518	1.245084
H	-8.121248	-2.365693	-1.499017	H	8.929428	-1.734933	2.075793
H	-7.047024	-3.781974	-1.309758	H	8.075377	-3.290270	1.859487

H	-6.314940	-1.612354	2.502792	H	7.433702	-1.366195	-2.101382
H	-4.339031	-0.113157	2.636313	H	5.302803	-0.147340	-2.480802
H	4.691858	0.351077	-1.037968	H	-3.223907	0.330746	-0.897320
H	2.498677	-0.140460	1.042619	H	-3.494681	-2.354736	0.533134
H	3.923413	1.362219	2.176747	H	-2.664657	-2.993073	-1.606839
H	5.505250	-0.628150	1.197109	H	-4.832723	-1.380010	-2.035407
H	4.787091	-1.544866	3.214959	H	-5.850288	-3.459646	-1.763748
H	3.220627	-2.646003	1.086414	H	-6.033539	-2.004831	0.699134
H	4.850003	-4.071500	1.468348	H	-7.922984	-1.678217	-0.372030
H	5.437713	-1.963033	-0.909917	H	-5.707487	0.632581	-0.819175
H	4.225509	-3.453943	-2.445995	H	-6.477926	1.687220	1.259743
H	4.811178	-4.341580	-1.027258	H	-7.727733	0.609740	0.612198
H	2.174649	-3.389432	-1.330005	H	-5.925054	-0.116073	2.652510
1b1				**1b1′**			
O	2.137354	0.363107	-0.320893	O	1.961885	0.309455	-0.500799
C	3.373453	1.109521	-0.287797	C	3.109936	1.158436	-0.286314
C	3.390969	2.027133	0.939819	C	2.860298	2.071724	0.919191
C	2.167097	2.921622	0.964172	C	1.583793	2.867297	0.732288
C	-0.261281	3.086653	0.420403	C	-0.732572	2.826819	-0.196531
C	-1.447684	2.533493	-0.087022	C	-1.776402	2.166268	-0.859905
C	-1.368598	1.237076	-0.615332	C	-1.529837	0.857769	-1.312405
C	-0.176720	0.491550	-0.726579	C	-0.268754	0.225995	-1.236528
C	0.982031	1.087200	-0.230449	C	0.747287	0.929353	-0.586091
C	0.966477	2.373271	0.362337	C	0.538652	2.213924	-0.032882
C	4.518085	0.125395	-0.318079	C	4.327506	0.279478	-0.129268
C	4.465140	-1.071757	0.398938	C	4.267810	-0.931717	0.562713
C	5.543137	-1.958947	0.407392	C	5.408135	-1.715708	0.749306
C	6.706028	-1.643901	-0.306238	C	6.639388	-1.280176	0.244622
C	6.770137	-0.444250	-1.029595	C	6.710780	-0.064841	-0.451594
C	5.685111	0.422220	-1.035731	C	5.565415	0.697543	-0.637370
O	-2.516358	0.669998	-1.155810	O	-2.552672	0.211507	-1.997878
C	-3.449193	0.134706	-0.262743	C	-3.512403	-0.548521	-1.294782
C	-4.779270	-0.029866	-0.999241	C	-3.033687	-1.954261	-0.901093
C	-5.759870	-0.797248	-0.113986	C	-4.099481	-2.646227	-0.052719
C	-5.162459	-2.115003	0.359400	C	-4.487779	-1.792062	1.143562
C	-3.829639	-1.833111	1.070845	C	-4.960206	-0.422566	0.634476
O	-2.964554	-1.139086	0.162777	O	-3.908809	0.170665	-0.138658
O	2.206015	4.041611	1.500473	O	1.452032	3.995216	1.235334
O	-0.312843	4.311743	0.965450	O	-0.963721	4.057478	0.290523
C	-2.715390	3.349571	-0.067131	C	-3.072846	2.897963	-1.093055
C	-0.130152	-0.875806	-1.358974	C	0.039303	-1.106618	-1.872694
O	7.817951	-2.431734	-0.366549	O	7.815167	-1.960623	0.369312
C	7.809530	-3.662034	0.341502	C	7.804220	-3.201839	1.057773
O	-5.291688	1.249864	-1.315970	O	-2.799417	-2.691900	-2.086994
O	-6.945138	-0.985796	-0.873432	O	-3.567681	-3.906146	0.332728

O	-6.124518	-2.716430	1.228177	O	-5.517771	-2.494785	1.840612
C	-3.077088	-3.094086	1.480691	C	-5.266249	0.569323	1.751458
O	-2.815677	-3.938777	0.372046	O	-4.156407	0.761349	2.611745
H	3.407157	1.735922	-1.191759	H	3.228255	1.787704	-1.181206
H	4.292004	2.645533	0.957211	H	3.696438	2.757879	1.075377
H	3.394264	1.415874	1.852332	H	2.761903	1.458987	1.825404
H	0.606323	4.520791	1.279452	H	-0.127124	4.345143	0.741280
H	-3.475328	2.924376	-0.723033	H	-3.676884	2.385267	-1.840785
H	-3.132578	3.422662	0.944868	H	-3.665976	2.981562	-0.176252
H	-2.501905	4.373964	-0.385312	H	-2.867559	3.917552	-1.431798
H	0.781108	-0.992440	-1.950500	H	0.926354	-1.020552	-2.508060
H	-0.124352	-1.666147	-0.598561	H	0.274858	-1.868335	-1.119644
H	-1.000294	-1.032160	-1.996278	H	-0.796467	-1.465667	-2.470332
H	3.561315	-1.327252	0.942486	H	3.313865	-1.279913	0.945000
H	5.464478	-2.883946	0.965826	H	5.324333	-2.655201	1.282252
H	8.782438	-4.120331	0.159345	H	8.832361	-3.565663	1.037914
H	7.679998	-3.507814	1.420278	H	7.483701	-3.083963	2.100732
H	7.021059	-4.333278	-0.021853	H	7.153094	-3.933704	0.563105
H	7.674663	-0.220579	-1.585028	H	7.670663	0.252848	-0.844590
H	5.745389	1.343149	-1.610659	H	5.634272	1.631938	-1.189201
H	-3.573693	0.787134	0.615354	H	-4.350817	-0.646628	-1.999626
H	-4.581123	-0.618917	-1.908143	H	-2.119632	-1.857410	-0.296818
H	-6.203011	1.108459	-1.611475	H	-2.653033	-3.607409	-1.806687
H	-5.974730	-0.180669	0.775607	H	-4.998378	-2.790156	-0.676410
H	-7.536761	-1.515975	-0.320072	H	-4.227153	-4.307736	0.916953
H	-4.964593	-2.757956	-0.506623	H	-3.613405	-1.640889	1.787742
H	-5.989124	-3.672078	1.207315	H	-5.494687	-2.217672	2.765193
H	-4.023152	-1.220918	1.967358	H	-5.862021	-0.560334	0.015465
H	-2.151105	-2.800186	1.995938	H	-5.604262	1.514427	1.302973
H	-3.685527	-3.667944	2.186975	H	-6.084811	0.179292	2.364910
H	-2.336355	-3.395685	-0.270823	H	-3.432609	1.086783	2.056766
1b1″				**1b2**			
O	2.288787	0.197128	-0.428931	O	-2.146835	0.281625	0.220606
C	3.378765	1.118006	-0.214265	C	-3.432984	0.887298	0.480338
C	3.141351	1.902354	1.081165	C	-3.612001	2.117287	-0.415073
C	1.793405	2.593499	1.051175	C	-2.461385	3.087762	-0.233902
C	-0.568049	2.445461	0.272374	C	-0.016329	3.314177	0.212054
C	-1.605030	1.772414	-0.395695	C	1.242180	2.739834	0.437629
C	-1.282996	0.546801	-0.998426	C	1.301114	1.343816	0.563757
C	0.023663	0.013576	-1.063386	C	0.174992	0.491127	0.527553
C	1.026014	0.721358	-0.403037	C	-1.055519	1.102815	0.281614
C	0.753865	1.927757	0.289842	C	-1.181452	2.501788	0.110359
C	4.666857	0.330497	-0.207667	C	-4.495493	-0.165586	0.278181
C	4.750232	-0.918782	0.410601	C	-4.442962	-1.048671	-0.802570
C	5.955052	-1.622448	0.461736	C	-5.448193	-1.993322	-1.016062

C	7.107332	-1.066458	-0.107327	C	-6.538047	-2.056276	-0.138832
C	7.034793	0.187182	-0.731435	C	-6.601126	-1.174884	0.949845
C	5.826308	0.869262	-0.782354	C	-5.587434	-0.247540	1.153047
O	-2.244078	-0.156077	-1.713257	O	2.563350	0.843913	0.833780
C	-3.240812	-0.939801	-1.104559	C	3.121726	-0.152430	0.016054
C	-2.937329	-1.440723	0.314754	C	4.400550	0.374850	-0.645176
C	-4.160417	-2.172905	0.868236	C	5.141366	-0.767952	-1.335040
C	-5.413028	-1.315260	0.788258	C	5.399329	-1.910460	-0.364048
C	-5.610616	-0.876187	-0.669501	C	4.060146	-2.359960	0.241053
O	-4.440260	-0.167618	-1.092115	O	3.439572	-1.236005	0.880928
O	1.606631	3.654170	1.671746	O	-2.627889	4.307658	-0.404688
O	-0.855798	3.597064	0.899769	O	-0.109587	4.644453	0.060687
C	-2.965754	2.416636	-0.468108	C	2.485274	3.588421	0.515926
C	0.321832	-1.246056	-1.835129	C	0.234865	-0.990546	0.809303
O	8.335449	-1.660718	-0.113720	O	-7.576153	-2.934028	-0.251912
C	8.468848	-2.935859	0.495242	C	-7.566157	-3.851668	-1.334818
O	-1.831010	-2.323089	0.274029	O	4.040225	1.370913	-1.584809
O	-3.843844	-2.543046	2.202971	O	6.343568	-0.226699	-1.863165
O	-6.493704	-2.114698	1.271916	O	6.034203	-2.953256	-1.105685
C	-6.783357	0.078054	-0.864416	C	4.209449	-3.423343	1.323537
O	-6.697894	1.216537	-0.023001	O	5.061973	-2.996645	2.372660
H	3.388586	1.826965	-1.055761	H	-3.440009	1.215423	1.530427
H	3.926373	2.644859	1.245269	H	-4.553353	2.629148	-0.199475
H	3.158913	1.209216	1.932947	H	-3.642205	1.802803	-1.466978
H	-0.010132	3.906894	1.321785	H	-1.063352	4.841604	-0.137257
H	-3.508930	2.064215	-1.344660	H	2.958419	3.506492	1.500532
H	-3.571572	2.194920	0.419941	H	3.217030	3.258756	-0.226649
H	-2.854955	3.502409	-0.512767	H	2.237682	4.635016	0.338389
H	-0.212927	-1.245217	-2.788594	H	-0.669235	-1.302328	1.336643
H	1.392273	-1.328862	-2.026056	H	0.281192	-1.588863	-0.110113
H	-0.006728	-2.128406	-1.278488	H	1.107045	-1.240574	1.413859
H	3.857274	-1.359951	0.841457	H	-3.594187	-1.014428	-1.478222
H	5.982173	-2.593858	0.940481	H	-5.370697	-2.668720	-1.859537
H	9.515715	-3.218092	0.375761	H	-8.475518	-4.445540	-1.233843
H	8.224508	-2.901874	1.564630	H	-7.578238	-3.335634	-2.303265
H	7.834898	-3.686522	0.006422	H	-6.694599	-4.517367	-1.294171
H	7.934686	0.598530	-1.176143	H	-7.447556	-1.243189	1.624871
H	5.782991	1.835488	-1.279175	H	-5.645043	0.422010	2.007787
H	-3.376477	-1.804081	-1.771685	H	2.406667	-0.468912	-0.757277
H	-2.730269	-0.571802	0.957235	H	5.038931	0.785353	0.151668
H	-1.782610	-2.727091	1.152996	H	4.844432	1.570797	-2.086022
H	-4.325184	-3.075515	0.255246	H	4.506363	-1.149377	-2.153021
H	-4.643471	-2.952853	2.563714	H	6.828803	-0.971692	-2.246386
H	-5.284731	-0.418814	1.406420	H	6.046615	-1.559391	0.448424
H	-7.174924	-1.519937	1.610428	H	6.568100	-3.473333	-0.491941
H	-5.768466	-1.769200	-1.297541	H	3.414638	-2.750794	-0.562767

H	-6.837869	0.358071	-1.926079	H	3.210325	-3.693930	1.694676
H	-7.712988	-0.439063	-0.606105	H	4.658930	-4.321601	0.888451
H	-5.875967	1.672078	-0.255398	H	4.677947	-2.176373	2.715607

Table S2. Optimized Z-Matrixes of **2** in the Gas Phase (Å).

2a1				**2a1′**			
O	-6.154178	-0.203048	0.117016	O	-4.832707	0.254865	-0.363040
C	-7.034207	-0.216591	-1.027777	C	-5.284426	-0.727861	0.591074
C	-7.463158	-1.655087	-1.335200	C	-6.054525	-0.041135	1.724262
C	-6.254944	-2.552073	-1.518456	C	-5.223687	1.056321	2.359816
C	-3.928498	-3.030648	-0.759147	C	-3.546922	2.852389	1.939684
C	-2.814749	-2.741201	0.043365	C	-2.703976	3.571884	1.076940
C	-2.884964	-1.591737	0.841854	C	-2.583855	3.102706	-0.240882
C	-4.001263	-0.729552	0.902569	C	-3.315806	2.007687	-0.755305
C	-5.076345	-1.041988	0.070559	C	-4.137178	1.322203	0.136410
C	-5.072103	-2.186999	-0.762186	C	-4.271031	1.716668	1.489384
C	-8.192286	0.709123	-0.743499	C	-6.102551	-1.761260	-0.145673
C	-8.812225	0.733406	0.507683	C	-7.000893	-1.394686	-1.150040
C	-9.910828	1.558293	0.755651	C	-7.793908	-2.345824	-1.794576
C	10.411748	2.372241	-0.267892	C	-7.699285	-3.693339	-1.425403
C	-9.797964	2.354754	-1.528573	C	-6.800338	-4.072846	-0.418244
C	-8.699672	1.535881	-1.755257	C	-6.011830	-3.115087	0.205627
O	-1.805474	-1.321911	1.675222	O	-1.798564	3.816350	-1.139448
C	-0.927399	-0.310836	1.275970	C	-0.455216	3.456301	-1.373287
C	-0.104643	0.133702	2.485607	C	0.538895	3.985002	-0.330460
C	0.983059	1.128580	2.042542	C	1.963089	3.498753	-0.656590
C	1.798390	0.510942	0.916867	C	1.950771	1.986308	-0.795118
C	0.877683	0.089241	-0.237716	C	0.923909	1.563018	-1.854655
O	-0.055970	-0.856588	0.282076	O	-0.356802	2.038683	-1.438538
O	-6.309894	-3.555314	-2.249223	O	-5.395773	1.378054	3.547908
O	-3.890880	-4.133234	-1.523981	O	-3.671596	3.281609	3.205721
C	-1.632696	-3.674262	0.027561	C	-2.040972	4.821909	1.595557
C	-4.075601	0.461966	1.826627	C	-3.263553	1.588939	-2.202418
O	11.477222	3.214272	-0.140180	O	-8.425375	-4.704503	-1.982644
C	12.130303	3.287857	1.118149	C	-9.351950	-4.381206	-3.008801
O	-0.949781	0.738165	3.441476	O	0.511259	5.397943	-0.343951
O	1.757444	1.511312	3.169399	O	2.861945	3.980255	0.331084
O	2.794687	1.413248	0.389848	O	3.233131	1.447288	-1.180988
C	1.627873	-0.551930	-1.414786	C	0.849555	0.041783	-2.050166
O	2.840851	-1.187655	-0.962136	O	1.216837	-0.646267	-0.837501
C	4.016771	-0.655111	-1.419664	C	2.347283	-1.418860	-0.894449
O	4.090693	0.126304	-2.338661	C	2.806410	-1.797201	0.478809
C	5.179141	-1.177768	-0.635087	C	1.835908	-2.224252	1.394586

C	6.242427	-0.321743	-0.255870	C	2.216779	-2.708054	2.639838
C	7.354357	-0.930776	0.343365	C	3.570946	-2.768345	2.968066
O	8.441948	-0.165919	0.698396	C	4.529607	-2.303618	2.067770
C	7.406637	-2.302942	0.588193	C	4.183947	-1.788779	0.810131
O	8.539583	-2.792098	1.178711	C	5.225047	-1.204398	-0.083553
C	6.320964	-3.113645	0.257577	C	6.341890	-1.954768	-0.484782
O	6.474218	-4.441809	0.564308	C	7.240817	-1.464161	-1.434924
C	5.208644	-2.550171	-0.354616	C	7.052078	-0.209232	-2.019883
C	6.182063	1.160142	-0.413199	C	5.970986	0.569072	-1.613727
C	7.182739	1.857122	-1.109205	C	5.091308	0.089929	-0.640354
O	8.326390	1.278277	-1.606500	C	4.012647	0.998810	-0.159654
C	7.058147	3.221033	-1.384271	O	2.886476	-1.747259	-1.924967
O	8.031591	3.896819	-2.063304	O	1.364337	-3.170800	3.609898
C	5.927753	3.934344	-0.977048	O	4.018031	-3.247190	4.168792
O	5.811367	5.261074	-1.251039	O	5.853184	-2.367095	2.438750
C	4.936574	3.273543	-0.255670	O	6.630582	-3.218845	-0.027698
C	5.077702	1.916945	0.045349	O	8.325753	-2.195804	-1.825523
C	4.044639	1.278180	0.908783	O	7.928510	0.260355	-2.947071
O	4.266407	0.680833	1.946720	O	3.812794	1.302554	1.002400
H	-6.464897	0.168098	-1.887282	H	-4.391847	-1.209312	1.019406
H	-8.087135	-1.698351	-2.231545	H	-6.353758	-0.760726	2.490710
H	-8.060184	-2.044152	-0.499424	H	-6.971938	0.408972	1.321603
H	-4.766814	-4.183603	-1.989844	H	-4.328384	2.680074	3.645199
H	-0.860753	-3.337856	0.716513	H	-1.532161	5.367217	0.802914
H	-1.943606	-4.689066	0.298087	H	-2.790513	5.472611	2.057366
H	-1.200634	-3.737358	-0.977038	H	-1.314103	4.589493	2.383147
H	-3.983900	1.407370	1.277778	H	-2.704562	0.656270	-2.332122
H	-5.046709	0.490624	2.328657	H	-4.272876	1.413367	-2.585503
H	-3.291685	0.427476	2.583199	H	-2.785252	2.358221	-2.807180
H	-8.420578	0.115152	1.309110	H	-7.070078	-0.353721	-1.448739
H	10.361345	1.560056	1.740828	H	-8.473106	-2.028215	-2.576470
H	12.934074	4.015316	0.997471	H	-9.816208	-5.323615	-3.302143
H	12.560107	2.320888	1.409081	H	10.127928	-3.692657	-2.651183
H	11.449686	3.629878	1.908097	H	-8.853037	-3.938282	-3.880025
H	10.192924	2.998469	-2.307282	H	-6.732971	-5.122033	-0.150968
H	-8.226579	1.542080	-2.734266	H	-5.312468	-3.425570	0.978355
H	-1.476321	0.543024	0.847181	H	-0.218397	3.906505	-2.349265
H	0.382193	-0.767210	2.892506	H	0.252407	3.582056	0.653113
H	-0.357942	1.154605	4.086798	H	1.255860	5.677699	0.210843
H	0.483130	2.036630	1.675587	H	2.265862	3.950402	-1.612183
H	2.615933	1.056594	3.119127	H	3.094697	3.241215	0.919025
H	2.308016	-0.382824	1.283501	H	1.661863	1.531657	0.155261
H	0.336525	0.970009	-0.621144	H	1.183410	2.016969	-2.825010
H	0.990983	-1.318389	-1.861713	H	-0.176673	-0.235444	-2.300966
H	1.889133	0.196629	-2.162803	H	1.523251	-0.277779	-2.845333
H	4.365372	-3.171503	-0.638164	H	0.787660	-2.193487	1.115702

H	5.672822	-4.929292	0.334929	H	0.447903	-3.040577	3.335153
H	8.412151	-3.738639	1.342408	H	3.247545	-3.465017	4.714662
H	9.079652	-0.746339	1.144451	H	5.889604	-2.693501	3.352370
H	8.696482	0.709277	-0.904913	H	6.521248	-3.212939	0.942334
H	8.729491	3.248750	-2.256363	H	8.296877	-3.021454	-1.313814
H	6.596358	5.526186	-1.754416	H	8.600884	-0.423744	-3.087969
H	4.073597	3.832254	0.086818	H	5.841180	1.555145	-2.043826
2a1″				**2a2**			
O	-3.995211	0.190082	0.486322	O	6.509407	0.123426	-0.133855
C	-4.241679	1.036953	-0.655680	C	7.648758	-0.684796	0.227509
C	-5.536592	0.594342	-1.342353	C	8.036166	-1.582781	-0.952184
C	-5.459427	-0.876877	-1.717236	C	6.851947	-2.406630	-1.416912
C	-4.498209	-3.103108	-1.116620	C	4.379226	-2.467790	-1.699643
C	-3.692478	-3.913965	-0.300922	C	3.112438	-1.867722	-1.606043
C	-2.992319	-3.287271	0.744154	C	3.049818	-0.618802	-0.968310
C	-3.149608	-1.922637	1.085555	C	4.173119	0.078581	-0.469950
C	-3.911693	-1.150081	0.211984	C	5.411948	-0.542887	-0.605119
C	-4.594119	-1.703370	-0.896029	C	5.543986	-1.819084	-1.209352
C	-4.229508	2.467103	-0.174819	C	8.760476	0.237211	0.667554
C	-4.938346	2.856754	0.963979	C	9.010731	1.440548	0.004653
C	-4.924749	4.178969	1.411567	C	10.071382	2.267210	0.380226
C	-4.191463	5.143650	0.708630	C	10.909724	1.883889	1.434164
C	-3.474147	4.765504	-0.437161	C	10.667251	0.677962	2.107328
C	-3.496595	3.442089	-0.867037	C	9.601935	-0.127776	1.727439
O	-2.165631	-4.092392	1.522843	O	1.855090	0.066709	-0.837697
C	-0.766309	-4.046340	1.337204	C	0.757259	-0.534760	-0.201951
C	-0.298439	-4.104953	-0.126292	C	0.332144	0.298439	1.010893
C	1.213856	-3.834723	-0.251964	C	-0.980513	-0.242837	1.601985
C	1.526722	-2.526920	0.450324	C	-2.024428	-0.310892	0.499956
C	1.110032	-2.627770	1.921854	C	-1.503001	-1.147036	-0.678307
O	-0.296655	-2.850516	1.954534	O	-0.302581	-0.536345	-1.155114
O	-6.127430	-1.325778	-2.662779	O	7.022706	-3.507626	-1.969966
O	-5.173657	-3.684140	-2.120574	O	4.472437	-3.663291	-2.302516
C	-3.663380	-5.398858	-0.555401	C	1.935574	-2.558110	-2.249906
C	-2.611756	-1.286902	2.344574	C	4.020540	1.423442	0.194586
O	-4.105315	6.457912	1.052807	O	11.975155	2.609009	1.882619
C	-4.809857	6.903379	2.204353	C	12.268677	3.839756	1.239644
O	-0.590600	-5.382555	-0.652313	O	1.351416	0.252574	1.989493
O	1.574559	-3.857392	-1.624572	O	-1.362831	0.559635	2.709284
O	2.918209	-2.149205	0.389494	O	-3.266462	-0.900330	0.941865
C	1.415496	-1.354976	2.718070	C	-2.500881	-1.241545	-1.843049
O	1.263285	-0.197145	1.870498	O	-3.373454	-0.093399	-1.864422
C	2.384681	0.566848	1.680528	C	-4.702808	-0.333310	-1.635889
O	3.367415	0.498411	2.380985	C	-5.436959	0.943171	-1.367756
C	2.227622	1.478017	0.503953	C	-5.161628	2.037397	-2.198331

C	3.306095	1.677520	-0.393589	C	-5.901224	3.207228	-2.079608
C	3.129734	2.662869	-1.374975	C	-6.919243	3.282197	-1.129237
O	4.155033	2.946893	-2.248351	C	-7.161733	2.203765	-0.278605
C	1.943854	3.386454	-1.492393	C	-6.424800	1.013098	-0.354679
O	1.877137	4.325235	-2.485429	C	-6.645322	-0.080714	0.634890
C	0.872632	3.125904	-0.636303	C	-7.915709	-0.651135	0.814923
O	-0.242386	3.886647	-0.871513	C	-8.098721	-1.769563	1.631646
C	1.016964	2.171708	0.364460	C	-7.018066	-2.359217	2.292772
C	4.550347	0.854264	-0.360313	C	-5.753274	-1.792226	2.157266
C	5.813274	1.456895	-0.248717	C	-5.578016	-0.655079	1.365338
O	6.026779	2.814994	-0.268473	C	-4.229053	-0.022824	1.333231
C	6.968243	0.692282	-0.067172	O	-5.202260	-1.433511	-1.657558
O	8.195683	1.281022	0.042623	O	-5.738798	4.333520	-2.845653
C	6.900476	-0.701053	0.013607	O	-7.696661	4.396102	-0.967499
O	8.028183	-1.438958	0.194538	O	-8.167479	2.324895	0.652975
C	5.664198	-1.325814	-0.130184	O	-9.059328	-0.205530	0.195653
C	4.515094	-0.560928	-0.344138	O	-9.334799	-2.323889	1.804093
C	3.233257	-1.273192	-0.604639	O	-7.202270	-3.449830	3.083322
O	2.515541	-1.093593	-1.572024	O	-3.990043	1.141740	1.598028
H	-3.411432	0.892357	-1.363552	H	7.350140	-1.325021	1.071134
H	-5.736628	1.183533	-2.241352	H	8.859823	-2.251120	-0.688014
H	-6.385108	0.736074	-0.659773	H	8.376109	-0.958549	-1.789472
H	-5.689087	-2.965396	-2.569725	H	5.440355	-3.895493	-2.319044
H	-4.686112	-5.790638	-0.557637	H	1.144022	-1.848791	-2.491279
H	-3.231306	-5.628352	-1.533404	H	2.262545	-3.056336	-3.165590
H	-3.077429	-5.914961	0.201481	H	1.511336	-3.340394	-1.607175
H	-1.732928	-0.664911	2.150989	H	3.272806	1.372150	0.990009
H	-3.379365	-0.643784	2.784666	H	4.972836	1.747740	0.614368
H	-2.325226	-2.049764	3.065790	H	3.684616	2.182047	-0.521505
H	-5.491798	2.112679	1.528089	H	8.356816	1.748717	-0.804769
H	-5.480339	4.442614	2.303269	H	10.230449	3.198851	-0.149382
H	-4.604096	7.971106	2.286373	H	13.145809	4.242753	1.747730
H	-5.891071	6.750552	2.099845	H	12.501954	3.696140	0.176938
H	-4.460072	6.397234	3.112671	H	11.439723	4.553094	1.331203
H	-2.913407	5.523955	-0.973376	H	11.320350	0.400990	2.928024
H	-2.935200	3.164765	-1.756045	H	9.420209	-1.054927	2.265532
H	-0.389335	-4.926144	1.877260	H	1.001926	-1.560834	0.110801
H	-0.824351	-3.313286	-0.682707	H	0.164405	1.326337	0.652574
H	-0.155646	-5.409893	-1.518617	H	0.966869	0.652693	2.784702
H	1.756748	-4.658757	0.231654	H	-0.789942	-1.254864	1.987798
H	1.649344	-2.937066	-1.931625	H	-2.120669	1.108263	2.442479
H	0.941820	-1.723900	-0.003199	H	-2.236564	0.695884	0.133153
H	1.634648	-3.466735	2.408628	H	-1.282573	-2.171122	-0.335405
H	0.709684	-1.271002	3.547383	H	-1.945326	-1.260108	-2.783167
H	2.435670	-1.372691	3.101841	H	-3.113427	-2.139016	-1.756592
H	0.203356	1.975072	1.054705	H	-4.381371	1.956519	-2.948210

H	-0.965794	3.664039	-0.267549	H	-4.998877	4.215549	-3.454774
H	0.990535	4.716358	-2.468434	H	-7.381958	5.077803	-1.580046
H	3.831265	3.609913	-2.879236	H	-8.521988	3.226586	0.591187
H	5.506187	3.182973	-1.007700	H	-9.077936	0.766980	0.278151
H	8.048332	2.237707	-0.043275	H	-9.951115	-1.785381	1.280167
H	8.772599	-0.822483	0.269689	H	-8.141847	-3.685471	3.043926
H	5.614588	-2.407928	-0.101189	H	-4.919780	-2.230803	2.693092
2b1				**2b1′**			
O	-5.550780	0.095770	-0.125660	O	-5.021027	-0.477251	-0.168996
C	-6.982040	0.049670	0.058080	C	-6.124407	0.010176	0.622908
C	-7.315260	-0.842250	1.258820	C	-5.598398	0.602306	1.935562
C	-6.703070	-2.218920	1.092690	C	-4.754874	-0.412663	2.682044
C	-4.775560	-3.513860	0.190740	C	-3.145198	-2.305072	2.444369
C	-3.545110	-3.581440	-0.483760	C	-2.374315	-3.166901	1.651854
C	-3.024700	-2.374450	-0.967230	C	-2.474682	-3.025201	0.257089
C	-3.679160	-1.127260	-0.886900	C	-3.387916	-2.154168	-0.379036
C	-4.908580	-1.107600	-0.231630	C	-4.150753	-1.330292	0.449841
C	-5.469620	-2.282110	0.332430	C	-4.031536	-1.361647	1.858909
C	-7.483540	1.466160	0.201320	C	-6.904544	1.000177	-0.208762
C	-6.793490	2.405770	0.970470	C	-6.265199	1.883032	-1.081061
C	-7.280620	3.703480	1.137480	C	-6.987002	2.830878	-1.809563
C	-8.488160	4.073690	0.532650	C	-8.376765	2.909739	-1.659629
C	-9.189770	3.138310	-0.241180	C	-9.029266	2.027337	-0.786445
C	-8.686050	1.854630	-0.405000	C	-8.297876	1.084031	-0.077280
O	-1.825640	-2.387810	-1.668510	O	-1.734370	-3.897505	-0.534460
C	-0.648630	-2.556840	-0.936240	C	-0.416348	-3.573694	-0.919229
C	0.464330	-2.984460	-1.893080	C	-0.318490	-2.560002	-2.068623
C	1.816430	-3.013610	-1.157380	C	1.150674	-2.196047	-2.353786
C	2.042170	-1.670620	-0.480430	C	1.813919	-1.753593	-1.061599
C	0.867340	-1.339970	0.452140	C	1.677649	-2.856067	-0.003044
O	-0.314500	-1.295450	-0.346650	O	0.283551	-3.075161	0.213693
O	-7.233340	-3.217060	1.609750	O	-4.680679	-0.393679	3.922555
O	-5.283920	-4.646370	0.699120	O	-3.022105	-2.385300	3.780396
C	-2.879270	-4.919730	-0.682970	C	-1.518914	-4.206465	2.326510
C	-3.079130	0.109580	-1.507150	C	-3.620759	-2.127991	-1.868973
O	-9.058400	5.309480	0.628030	O	-9.180481	3.795900	-2.315244
C	-8.390230	6.302010	1.391520	C	-8.576973	4.712283	-3.215753
O	0.172070	-4.262540	-2.417040	O	-0.891062	-3.129431	-3.229411
O	2.840810	-3.376740	-2.070460	O	1.199459	-1.225174	-3.388871
O	3.258360	-1.632180	0.297510	O	3.216888	-1.455402	-1.223869
C	1.028570	0.002010	1.179120	C	2.338382	-2.498703	1.335643
O	1.811790	0.918380	0.387150	O	2.334512	-1.071631	1.538905
C	3.012780	1.308270	0.918150	C	3.558916	-0.459475	1.587331
O	3.323690	1.142340	2.074200	O	4.603935	-1.052267	1.717562
C	3.867400	1.964450	-0.120510	C	3.415921	1.025012	1.464398

C	5.257400	1.699710	-0.188960	C	4.321131	1.779128	0.677722
C	5.998690	2.471480	-1.095310	C	4.197291	3.174389	0.745102
O	7.361170	2.298970	-1.182060	O	5.071897	3.971678	0.042288
C	5.402400	3.428250	-1.916580	C	3.216307	3.795929	1.517694
O	6.219630	4.123470	-2.765200	O	3.185737	5.163693	1.511215
C	4.022660	3.626690	-1.870130	C	2.301246	3.027077	2.236688
O	3.543330	4.576060	-2.736690	O	1.368082	3.744098	2.941157
C	3.256800	2.895170	-0.971270	C	2.402277	1.642035	2.209373
C	5.912910	0.618590	0.602260	C	5.320530	1.147432	-0.231609
C	7.007060	0.894220	1.437950	C	6.686530	1.458254	-0.135898
O	7.626480	2.118620	1.523290	O	7.205927	2.416815	0.701485
C	7.528690	-0.079450	2.292960	C	7.641642	0.764335	-0.882738
O	8.591510	0.190270	3.107200	O	8.969900	1.067572	-0.788088
C	6.972310	-1.360240	2.345250	C	7.265300	-0.267172	-1.746876
O	7.482380	-2.301910	3.182790	O	8.200283	-0.940641	-2.468533
C	5.908580	-1.669220	1.501090	C	5.913523	-0.572645	-1.884836
C	5.408790	-0.703730	0.624240	C	4.957649	0.143890	-1.161249
C	4.342860	-1.108830	-0.335280	C	3.518877	-0.143651	-1.421995
O	4.399060	-0.976340	-1.544730	O	2.685411	0.680715	-1.752265
H	-7.420280	-0.401300	-0.844800	H	-6.767044	-0.850333	0.862855
H	-8.395630	-0.940670	1.392180	H	-6.419308	0.933653	2.576554
H	-6.910670	-0.388350	2.173450	H	-4.977213	1.480850	1.714572
H	-6.136180	-4.397630	1.146690	H	-3.618196	-1.688801	4.160825
H	-2.122590	-4.877510	-1.467270	H	-1.182026	-4.955645	1.611295
H	-2.403530	-5.278810	0.238240	H	-0.636206	-3.758294	2.794371
H	-3.629360	-5.668470	-0.952120	H	-2.087146	-4.696744	3.122516
H	-2.812710	-0.073230	-2.552600	H	-4.689807	-2.227525	-2.081281
H	-3.785530	0.938600	-1.462420	H	-3.308021	-1.173688	-2.309833
H	-2.157570	0.398320	-0.993590	H	-3.077151	-2.925694	-2.370795
H	-5.850170	2.128440	1.430070	H	-5.190054	1.817500	-1.211361
H	-6.715400	4.410310	1.732930	H	-6.460490	3.492985	-2.486373
H	-9.012110	7.196220	1.332170	H	-9.389890	5.318537	-3.617526
H	-8.287020	6.004030	2.442650	H	-7.857270	5.365779	-2.706483
H	-7.396490	6.526270	0.983270	H	-8.070578	4.195739	-4.040997
H	10.118750	3.444690	-0.710060	H	10.107670	2.094747	-0.690196
H	-9.235210	1.143550	-1.017300	H	-8.819179	0.399259	0.587346
H	-0.780660	-3.303200	-0.137470	H	0.012223	-4.531095	-1.251123
H	0.512140	-2.225170	-2.690330	H	-0.846453	-1.643450	-1.762554
H	0.980710	-4.552150	-2.866740	H	-0.679249	-2.517922	-3.951462
H	1.772350	-3.804580	-0.394860	H	1.656002	-3.095248	-2.734319
H	3.348220	-2.577230	-2.293140	H	1.401277	-0.362878	-2.986498
H	2.098800	-0.885300	-1.237620	H	1.316975	-0.858712	-0.680334
H	0.766200	-2.126980	1.217800	H	2.141642	-3.785862	-0.370907
H	0.040970	0.442760	1.332890	H	1.770979	-2.959130	2.147274
H	1.525760	-0.135310	2.139410	H	3.370546	-2.848558	1.361358
H	2.185140	3.053880	-0.908180	H	1.710832	1.030462	2.779886

H	2.581080	4.625640	-2.673420	H	0.767660	3.144162	3.401897
H	5.667540	4.700250	-3.314280	H	2.431520	5.452661	2.046615
H	7.688170	2.872840	-1.893580	H	4.799688	4.894711	0.170397
H	7.768780	2.439360	0.612420	H	6.650856	3.215082	0.614196
H	8.843120	1.112380	2.932140	H	9.037941	1.802230	-0.155672
H	8.207760	-1.891640	3.678140	H	9.068481	-0.578996	-2.233328
H	5.496250	-2.671140	1.518770	H	5.618156	-1.351977	-2.577391
2b1″				**2b2**			
O	-6.055819	-0.034320	0.326279	O	5.902550	0.018621	0.294271
C	-7.109705	0.926531	0.112904	C	7.314252	-0.122773	0.566653
C	-6.638659	1.991546	-0.883694	C	7.976814	-0.922945	-0.559138
C	-5.349288	2.634337	-0.413237	C	7.285022	-2.258473	-0.748625
C	-3.203240	2.278377	0.801140	C	5.102117	-3.466137	-0.682720
C	-2.310039	1.458331	1.512001	C	3.712637	-3.467786	-0.498957
C	-2.708179	0.131004	1.731431	C	3.117658	-2.272782	-0.067706
C	-3.971922	-0.390587	1.376040	C	3.830862	-1.092566	0.241382
C	-4.837394	0.463948	0.697633	C	5.209184	-1.128318	0.023793
C	-4.470177	1.795862	0.378281	C	5.868374	-2.289589	-0.445014
C	-8.341662	0.182297	-0.343695	C	7.898222	1.257342	0.748513
C	-8.252722	-0.903621	-1.216917	C	7.530765	2.316296	-0.084570
C	-9.397057	-1.559176	-1.675686	C	8.107548	3.580119	0.053091
C	10.660706	-1.118486	-1.264257	C	9.080709	3.794728	1.036974
C	10.761601	-0.028629	-0.387591	C	9.457015	2.738884	1.879415
C	-9.613229	0.605793	0.067186	C	8.865834	1.490568	1.735440
O	-1.905675	-0.732799	2.465833	O	1.751439	-2.351770	0.137560
C	-0.753694	-1.347291	1.947553	C	0.887985	-1.445484	-0.498748
C	-0.667678	-1.460526	0.420522	C	-0.063922	-2.192968	-1.438394
C	0.683663	-2.076703	0.008241	C	-1.142439	-1.241736	-1.982658
C	1.812899	-1.282061	0.641433	C	-1.834319	-0.566939	-0.810332
C	1.628870	-1.232475	2.164172	C	-0.804170	0.143876	0.079317
O	0.373308	-0.609046	2.425224	O	0.131547	-0.831576	0.541474
O	-5.073124	3.806840	-0.721861	O	7.913457	-3.245274	-1.168793
O	-2.832576	3.540629	0.528591	O	5.704712	-4.583148	-1.119135
C	-1.023566	2.048717	2.029632	C	2.888569	-4.697890	-0.780129
C	-4.364433	-1.799977	1.737257	C	3.195987	0.135077	0.848211
O	11.843252	-1.679739	-1.649374	O	9.711753	4.983650	1.259085
C	11.804275	-2.792430	-2.529773	C	9.369569	6.090224	0.438505
O	-1.716560	-2.276387	-0.060056	O	0.677177	-2.739218	-2.510752
O	0.746918	-2.140201	-1.408289	O	-2.021561	-1.962955	-2.832837
O	3.117503	-1.835464	0.363241	O	-2.810354	0.413693	-1.223331
C	2.730735	-0.441301	2.882196	C	-1.432876	0.835352	1.298792
O	3.256604	0.587732	2.019593	O	-2.653380	0.173614	1.688973
C	4.572411	0.465635	1.657741	C	-3.806424	0.905094	1.576781
C	4.895131	1.365929	0.506894	C	-5.010839	0.023512	1.685763
C	4.393750	2.673811	0.543267	C	-5.015088	-0.949769	2.693499

C	4.762936	3.589874	-0.433559	C	-6.154759	-1.709681	2.924895
C	5.639080	3.198267	-1.445829	C	-7.292926	-1.493724	2.148148
C	6.103249	1.884016	-1.498870	C	-7.268741	-0.551835	1.119633
C	5.736142	0.924571	-0.544588	C	-6.131837	0.220614	0.842187
C	6.165054	-0.496222	-0.692908	C	-6.107496	1.142726	-0.329734
C	7.523122	-0.838539	-0.790602	C	-7.067331	2.156940	-0.475911
C	7.936324	-2.172987	-0.780963	C	-6.963472	3.111781	-1.490383
C	7.007016	-3.210580	-0.669951	C	-5.895262	3.087842	-2.390991
C	5.651094	-2.898705	-0.607647	C	-4.948331	2.071854	-2.288191
C	5.238366	-1.565075	-0.649188	C	-5.070978	1.100017	-1.292506
C	3.776160	-1.281767	-0.690582	C	-4.096039	-0.026719	-1.286500
O	5.355647	-0.272778	2.207295	O	-3.831199	2.102856	1.417501
O	4.355007	4.897765	-0.494267	O	-6.286186	-2.674699	3.890741
O	6.056031	4.051476	-2.430138	O	-8.453899	-2.193912	2.329797
O	6.953749	1.536050	-2.523287	O	-8.408880	-0.381309	0.368199
O	8.548213	0.074579	-0.864204	O	-8.145698	2.328689	0.359284
O	9.257997	-2.504092	-0.873897	O	-7.896722	4.098842	-1.630016
O	7.416173	-4.507220	-0.657783	O	-5.798432	4.021947	-3.374106
O	3.213230	-0.616089	-1.541377	O	-4.386191	-1.209275	-1.310598
H	-7.316347	1.416769	1.076274	H	7.417173	-0.688652	1.504621
H	-7.397322	2.765229	-1.026960	H	9.037172	-1.090256	-0.353825
H	-6.459052	1.521218	-1.859822	H	7.907958	-0.357542	-1.498145
H	-3.580532	3.947498	0.014075	H	6.666748	-4.360814	-1.232586
H	-0.683763	1.517199	2.917482	H	2.391929	-5.056861	0.128003
H	-0.214778	1.996400	1.291257	H	2.108214	-4.472118	-1.511856
H	-1.176637	3.104360	2.265096	H	3.523833	-5.496086	-1.164246
H	-4.126878	-2.009173	2.784168	H	2.274522	-0.119675	1.372655
H	-5.432669	-1.949756	1.579247	H	3.890909	0.601431	1.549944
H	-3.811574	-2.519896	1.126836	H	2.955851	0.897612	0.095559
H	-7.275350	-1.257492	-1.528302	H	6.767977	2.159552	-0.840495
H	-9.291483	-2.405510	-2.343663	H	7.792325	4.381698	-0.604058
H	12.843372	-3.076426	-2.701560	H	9.985681	6.921828	0.782992
H	11.337916	-2.534223	-3.489059	H	9.588016	5.893337	-0.618763
H	11.267076	-3.640802	-2.087065	H	8.310618	6.359065	0.541873
H	11.747900	0.293257	-0.070741	H	10.205348	2.924861	2.642426
H	-9.706662	1.442370	0.755494	H	9.160184	0.684279	2.402852
H	-0.736220	-2.354609	2.391436	H	1.458472	-0.692617	-1.063080
H	-0.727531	-0.445494	-0.001838	H	-0.551041	-2.981180	-0.842831
H	-1.517939	-2.426938	-0.997195	H	0.018662	-3.057624	-3.147299
H	0.711707	-3.111401	0.379235	H	-0.646953	-0.480913	-2.603074
H	1.358836	-1.449285	-1.717001	H	-2.860652	-2.098659	-2.359704
H	1.793493	-0.256112	0.267132	H	-2.343444	-1.319808	-0.204469
H	1.624599	-2.256983	2.572291	H	-0.274967	0.911196	-0.509337
H	2.303570	0.039649	3.764933	H	-0.734233	0.778090	2.136379
H	3.550098	-1.096978	3.177150	H	-1.661938	1.877800	1.077625
H	3.732236	2.970467	1.350607	H	-4.129202	-1.090231	3.304245

H	3.695789	5.072147	0.189590	H	-5.449859	-2.790283	4.359414
H	5.603106	4.899512	-2.308069	H	-8.307408	-2.849320	3.028346
H	7.042926	2.305497	-3.108535	H	-9.060891	-1.036405	0.665307
H	8.290599	0.753491	-1.516584	H	-8.553868	1.452502	0.496039
H	9.744473	-1.666302	-0.949920	H	-8.556277	3.951837	-0.931601
H	8.384202	-4.509675	-0.710508	H	-6.546503	4.630597	-3.275027
H	4.927726	-3.703728	-0.553580	H	-4.136667	2.034723	-3.005128

Table S3. Optimized Z-Matrixes of **3** in the Gas Phase (Å).

3a1				**3b1**			
O	5.598317	-0.239049	-0.177279	O	5.627673	0.198350	-0.233997
C	6.339565	0.658584	0.676863	C	6.945864	0.065914	0.337570
C	7.061473	-0.140398	1.766972	C	6.826462	-0.245301	1.833463
C	6.085767	-1.006708	2.538523	C	5.989682	0.805337	2.535851
C	4.027005	-2.405135	2.383426	C	4.066108	2.374591	2.326795
C	2.966401	-2.950755	1.644708	C	3.016450	2.944412	1.587280
C	2.843870	-2.544519	0.309223	C	2.871500	2.509905	0.263729
C	3.723113	-1.648466	-0.336657	C	3.739720	1.608804	-0.387121
C	4.750788	-1.114920	0.440962	C	4.783836	1.087072	0.373680
C	4.932596	-1.480221	1.796711	C	4.957236	1.437725	1.737332
C	7.272162	1.471056	-0.188641	C	7.693141	-0.992195	-0.438064
C	7.979248	0.886391	-1.241436	C	7.057225	-2.152469	-0.884276
C	8.877677	1.628225	-2.010436	C	7.762155	-3.150075	-1.560750
C	9.085897	2.982258	-1.719993	C	9.134784	-2.995175	-1.790079
C	8.381709	3.579479	-0.664609	C	9.783760	-1.834429	-1.344972
C	7.483950	2.829532	0.083717	C	9.065754	-0.847297	-0.683250
O	1.825696	-3.117516	-0.444930	O	1.868380	3.060595	-0.524653
C	0.687305	-2.341487	-0.679415	C	0.555877	2.649608	-0.281808
C	-0.078817	-2.954368	-1.854016	C	-0.389737	3.654333	-0.942936
C	-1.451967	-2.280256	-2.019183	C	-1.841312	3.144438	-0.904791
C	-2.192725	-2.291151	-0.680155	C	-1.900382	1.719827	-1.462310
C	-1.307386	-1.587838	0.374058	C	-0.932987	0.834204	-0.643348
O	-0.123661	-2.381166	0.495378	O	0.377520	1.359622	-0.872732
O	6.301372	-1.310154	3.723843	O	6.179853	1.072958	3.734742
O	4.172429	-2.785803	3.662368	O	4.210317	2.739058	3.609890
C	2.043806	-3.943770	2.300811	C	2.142498	3.994834	2.225034
C	3.604164	-1.282361	-1.796325	C	3.550696	1.256755	-1.841277
O	9.938350	3.800866	-2.401046	O	9.922031	-3.902418	-2.436794
C	10.667637	3.256470	-3.490642	C	9.317051	-5.089018	-2.927436
O	0.677569	-2.813881	-3.037789	O	-0.291164	4.897593	-0.281802
O	-2.167556	-2.895052	-3.085999	O	-2.696296	4.067190	-1.571763
O	-3.551134	-1.835316	-0.757927	O	-3.231071	1.206221	-1.621973
C	-1.936213	-1.451570	1.769954	C	-0.927321	-0.655680	-1.021115

O	-2.464346	-0.117365	1.880352	O	-1.752052	-1.348344	-0.066771
C	-3.843458	-0.527943	-1.011652	C	-4.007870	0.917703	-0.539076
O	-3.001480	0.320181	-1.224964	O	-3.657154	1.106285	0.607804
C	-5.319513	-0.322549	-0.945411	C	-5.296032	0.315386	-0.989090
C	-6.116923	-1.290765	-1.566141	C	-5.919442	0.910288	-2.091829
C	-7.501378	-1.170604	-1.579548	C	-7.136182	0.432952	-2.564449
O	-8.272104	-2.100227	-2.206976	O	-7.752322	1.030232	-3.620611
C	-8.082013	-0.068096	-0.951680	C	-7.720718	-0.658907	-1.921489
O	-9.441616	0.046209	-0.977857	O	-8.920838	-1.113262	-2.385540
C	-7.292055	0.891209	-0.312572	C	-7.092828	-1.269916	-0.832770
O	-8.019310	1.890664	0.295823	O	-7.775970	-2.359450	-0.338839
C	-5.888420	0.793405	-0.279323	C	-5.858166	-0.812064	-0.336714
C	-5.097758	1.801719	0.491876	C	-5.188082	-1.556501	0.773702
C	-5.284967	3.172467	0.242601	C	-5.892152	-1.817690	1.961702
O	-6.211330	3.586239	-0.691098	O	-7.204305	-1.414986	2.091182
C	-4.572806	4.162488	0.918625	C	-5.320251	-2.491434	3.040219
O	-4.849900	5.464605	0.596486	O	-6.108531	-2.694637	4.141507
C	-3.609236	3.810066	1.859984	C	-3.992652	-2.907038	2.979702
O	-2.958823	4.862210	2.454453	O	-3.528315	-3.547596	4.101077
C	-3.381175	2.466774	2.123989	C	-3.257325	-2.656502	1.829566
C	-4.124518	1.477059	1.468440	C	-3.846930	-2.010527	0.735442
C	-3.818128	0.055027	1.822509	C	-2.982694	-1.787062	-0.466201
O	-4.621212	-0.828294	2.010580	O	-3.302965	-1.939656	-1.621573
H	5.613889	1.330275	1.159809	H	7.458825	1.032493	0.221713
H	7.586279	0.521768	2.460301	H	7.809865	-0.300534	2.307289
H	7.812979	-0.792946	1.302572	H	6.342472	-1.222596	1.963718
H	4.984678	-2.327042	4.003313	H	4.984499	2.225340	3.963947
H	1.345509	-4.362480	1.578881	H	1.600950	4.573612	1.475786
H	2.620775	-4.752181	2.760995	H	1.412200	3.553406	2.914686
H	1.467743	-3.472121	3.104550	H	2.757556	4.673569	2.822152
H	3.221230	-0.262952	-1.929141	H	3.498297	2.161294	-2.455078
H	4.587580	-1.306921	-2.273952	H	4.376982	0.639836	-2.194153
H	2.941273	-1.967322	-2.324938	H	2.611721	0.717095	-1.994087
H	7.812865	-0.159192	-1.479878	H	5.991129	-2.271605	-0.720405
H	9.402096	1.145615	-2.826280	H	7.235351	-4.032585	-1.903485
H	11.272103	4.073897	-3.885911	H	10.115093	-5.657222	-3.407120
H	11.329165	2.441971	-3.169216	H	8.884885	-5.689122	-2.116550
H	10.000647	2.886733	-4.279664	H	8.536059	-4.869329	-3.666371
H	8.547876	4.631613	-0.459228	H	10.845380	-1.726012	-1.539831
H	6.936432	3.308902	0.891692	H	9.580149	0.052569	-0.354756
H	0.956933	-1.297004	-0.900778	H	0.350902	2.582100	0.796897
H	-0.233596	-4.018912	-1.602792	H	-0.070009	3.735346	-1.997334
H	0.058941	-2.968692	-3.768155	H	-1.072374	5.404980	-0.550702
H	-1.303934	-1.245294	-2.339843	H	-2.188851	3.138979	0.131904
H	-2.442951	-3.777968	-2.797800	H	-2.515157	4.017363	-2.522089
H	-2.309503	-3.328855	-0.343599	H	-1.521492	1.721712	-2.491859

H	-1.052579	-0.577893	0.031117	H	-1.183249	0.897267	0.422499
H	-2.727177	-2.179489	1.961781	H	-1.290819	-0.848504	-2.032655
H	-1.145944	-1.550540	2.516704	H	0.089328	-1.037667	-0.908303
H	-5.658528	-2.140964	-2.055029	H	-5.462502	1.760510	-2.582079
H	-9.197970	-1.837125	-2.092176	H	-8.575039	0.546402	-3.789948
H	-9.649350	0.864245	-0.494448	H	-9.159820	-1.864330	-1.815614
H	-7.636394	2.742204	0.007944	H	-7.846829	-2.240844	0.628411
H	-6.138243	4.551694	-0.766092	H	-7.484998	-1.621168	2.997705
H	-4.239210	6.034295	1.087549	H	-5.565036	-3.103743	4.831425
H	-2.279302	4.531433	3.055428	H	-2.587050	-3.739947	4.004285
H	-2.622469	2.174054	2.842240	H	-2.217172	-2.959566	1.771272

Table S4. Optimized Z-Matrixes of **4** in the Gas Phase (Å).

4a1				**4b1**			
O	-5.666603	0.230358	-0.143488	O	-5.505326	-0.257771	-0.275828
C	-6.381265	-0.820498	0.541661	C	-6.847447	-0.132763	0.246684
C	-7.063837	-0.248440	1.788627	C	-6.798128	-0.022914	1.774369
C	-6.059329	0.453754	2.679598	C	-6.046031	-1.193779	2.375861
C	-3.982823	1.827433	2.742205	C	-4.155885	-2.792013	2.062824
C	-2.935639	2.504720	2.096102	C	-3.064404	-3.272075	1.321659
C	-2.847096	2.351579	0.706012	C	-2.840593	-2.690449	0.067397
C	-3.744763	1.598088	-0.077581	C	-3.653916	-1.687859	-0.505008
C	-4.779248	0.954656	0.601588	C	-4.722413	-1.235141	0.269465
C	-4.918844	1.050184	2.009154	C	-4.989316	-1.758096	1.557013
C	-7.345201	-1.449844	-0.434972	C	-7.503186	1.051456	-0.421224
C	-8.051991	-0.677532	-1.359031	C	-6.803282	2.239835	-0.641147
C	-8.978018	-1.256684	-2.228743	C	-7.423838	3.350021	-1.216580
C	-9.214986	-2.635608	-2.171561	C	-8.776251	3.281001	-1.573572
C	-8.510850	-3.420516	-1.246823	C	-9.488761	2.092700	-1.357125
C	-7.585761	-2.830310	-0.396231	C	-8.853474	0.994262	-0.793190
O	-1.856931	3.034818	0.005796	O	-1.797838	-3.213501	-0.692559
C	-0.533246	2.579345	0.120925	C	-0.636178	-2.435899	-0.828269
C	0.368151	3.690660	-0.418128	C	0.188561	-3.056971	-1.956737
C	1.832181	3.239744	-0.456865	C	1.543338	-2.354390	-2.095556
C	1.904352	1.911417	-1.212739	C	2.217452	-2.342835	-0.721988
C	0.957371	0.882913	-0.553227	C	1.281526	-1.677611	0.312242
O	-0.374000	1.406093	-0.668527	O	0.099068	-2.486302	0.387418
O	-6.239853	0.530746	3.906641	O	-6.314595	-1.608485	3.515305
O	-4.096939	1.959541	4.072177	O	-4.382229	-3.317554	3.276052
C	-2.019119	3.379930	2.914054	C	-2.204070	-4.369283	1.891951
C	-3.598389	1.502460	-1.575525	C	-3.450147	-1.140121	-1.896518
O	10.095970	-3.306538	-2.967467	O	-9.483575	4.300827	-2.138483
C	10.833590	-2.566350	-3.928585	C	-8.812548	5.525871	-2.392584

O	0.314032	4.862835	0.385124	O	-0.463071	-2.959686	-3.217318
O	2.631302	4.194219	-1.130515	O	2.374471	-3.046623	-3.008392
O	3.241883	1.436409	-1.428396	O	3.556257	-1.824648	-0.732875
C	0.979921	-0.516772	-1.187795	C	1.866510	-1.552094	1.727856
O	1.805088	-1.354367	-0.357662	O	2.338347	-0.200572	1.881068
C	4.015052	0.995943	-0.399841	C	3.810313	-0.509947	-0.968716
O	3.659410	0.990485	0.761843	O	2.951207	0.314759	-1.209461
C	5.319582	0.502469	-0.932171	C	5.276888	-0.257231	-0.849657
C	5.937995	1.292993	-1.907654	C	6.124556	-1.190869	-1.456778
C	7.169608	0.928981	-2.439816	C	7.504109	-1.022970	-1.425058
O	7.783496	1.712156	-3.368202	O	8.326250	-1.916867	-2.038955
C	7.771820	-0.246277	-1.989068	C	8.027454	0.090143	-0.766017
O	8.986108	-0.589795	-2.510405	O	9.383206	0.250846	-0.748367
C	7.147909	-1.050511	-1.032029	C	7.186476	1.012975	-0.139138
O	7.849530	-2.197381	-0.728679	O	7.859636	2.028101	0.505965
C	5.899668	-0.709794	-0.478586	C	5.786763	0.867232	-0.151653
C	5.235210	-1.649678	0.475944	C	4.938256	1.835877	0.608242
C	5.934174	-2.105002	1.607307	C	5.083635	3.216151	0.384759
O	7.236497	-1.707010	1.823229	O	6.022899	3.677030	-0.513355
C	5.367554	-2.972230	2.540644	C	4.316409	4.169502	1.053098
O	6.150672	-3.355660	3.597288	O	4.556035	5.486246	0.759133
C	4.049295	-3.394843	2.391183	C	3.338655	3.768484	1.959551
O	3.588559	-4.234854	3.374578	O	2.632745	4.787683	2.549678
C	3.318189	-2.955784	1.296356	C	3.151081	2.414136	2.197190
C	3.903997	-2.114488	0.341828	C	3.949073	1.461881	1.550352
C	3.045788	-1.701999	-0.813696	C	3.685989	0.024406	1.878176
O	3.376461	-1.655282	-1.974832	O	4.515197	-0.827787	2.092032
H	-5.643070	-1.571681	0.860561	H	-7.393049	-1.050149	-0.019942
H	-7.826708	0.480672	1.484115	H	-6.283221	0.905167	2.056976
H	-7.569341	-1.031940	2.358897	H	-7.804083	0.018412	2.199599
H	-4.912863	1.456025	4.337232	H	-5.156172	-2.826288	3.658603
H	-1.329369	2.784975	3.524776	H	-2.722958	-5.334559	1.851675
H	-1.425296	4.045890	2.287865	H	-1.265856	-4.454574	1.347411
H	-2.605649	3.983485	3.612554	H	-1.989062	-4.172718	2.945908
H	-4.195672	0.675641	-1.961323	H	-4.409032	-1.066039	-2.416485
H	-3.941557	2.421059	-2.066775	H	-3.027499	-0.128041	-1.879429
H	-2.553695	1.354937	-1.853344	H	-2.779428	-1.768220	-2.482690
H	-7.862922	0.389496	-1.416549	H	-5.751382	2.295407	-0.379752
H	-9.501034	-0.629587	-2.940622	H	-6.848270	4.252638	-1.382810
H	10.173887	-2.080349	-4.658532	H	-7.977484	5.392379	-3.091870
H	11.466803	-3.289877	-4.443626	H	-9.554404	6.187270	-2.841891
H	11.466858	-1.805645	-3.454780	H	-8.436712	5.981193	-1.467512
H	-8.699475	-4.488499	-1.222593	H	10.532872	2.053012	-1.648584
H	-7.039609	-3.453747	0.307612	H	-9.416212	0.076145	-0.642616
H	-0.286993	2.346460	1.167613	H	-0.888898	-1.389089	-1.057470
H	0.043057	3.902358	-1.447250	H	0.369332	-4.107623	-1.686996

H	-0.570330	5.239755	0.280808	H	-1.226694	-3.552080	-3.190176
H	2.183651	3.090600	0.573810	H	1.374057	-1.319714	-2.425753
H	2.482341	5.035627	-0.675500	H	1.867999	-3.115901	-3.830558
H	1.545292	2.080813	-2.232949	H	2.368137	-3.380689	-0.408213
H	1.216223	0.763405	0.505273	H	1.017266	-0.666911	-0.020516
H	1.361444	-0.521748	-2.210795	H	2.681318	-2.251967	1.923595
H	-0.031206	-0.928273	-1.161591	H	1.062297	-1.700026	2.451467
H	5.463183	2.204342	-2.249234	H	5.708845	-2.050953	-1.966822
H	8.615832	1.278504	-3.610414	H	9.238214	-1.625168	-1.888116
H	9.234068	-1.424530	-2.077313	H	9.547139	1.067748	-0.246771
H	7.909616	-2.248815	0.245003	H	7.456591	2.869683	0.217128
H	7.512863	-2.068057	2.681257	H	5.920239	4.640784	-0.572845
H	5.609719	-3.894346	4.193780	H	3.916487	6.025733	1.247406
H	2.655311	-4.433081	3.226290	H	1.960577	4.422311	3.138685
H	2.284871	-3.262690	1.172585	H	2.382271	2.083509	2.887862

Table S5: Important Thermodynamic Parameters of Compound **1** (au).

species	in gas phase						in MeOH
	E	*E′=E+ZPE*	*H*	*G*	E_{lbs}	*Ew*	E_s
1a1	-1683.670741	-1683.168707	-1683.135254	-1683.233946	-1684.117687	-1683.040046	-1683.702546
1a1′	-1683.664255	-1683.161946	-1683.128763	-1683.226633	-1684.110253	-1683.033424	-1683.700107
1a1″	-1683.663498	-1683.161737	-1683.128199	-1683.227552	-1684.109628	-1683.032384	-1683.698869
1a2	-1683.669496	-1683.167092	-1683.133847	-1683.231843	-1684.115736	-1683.038881	-1683.701602
1b1	-1683.670977	-1683.169000	-1683.135539	-1683.234500	-1684.117859	-1683.040292	-1683.702745
1b1′	-1683.664629	-1683.162339	-1683.129140	-1683.226948	-1684.110636	-1683.033831	-1683.700428
1b1″	-1683.664632	-1683.162549	-1683.129227	-1683.227548	-1684.110613	-1683.033538	-1683.695274
1b2	-1683.668929	-1683.166600	-1683.133310	-1683.231640	-1684.115225	-1683.038293	-1683.701359

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at the B3LYP/6-31G** level; E_{lbs}: single point energy in the gas phase at the B3LYP/6-311 ++G**//B3LYP/6-31G** level; E_w: single point energy at the B3PW91/6-31G**//B3LYP/6-31G** level; E_s: single point energy in MeOH solution at the B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model.

Table S6. Conformational Analysis of Compound **1**.

species	in gas phase										in MeOH	
	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$	$\Delta E_{lbs}{}^g$	$P_{Elbs}\%^h$	ΔEw^i	$P_{Ew}\%^j$	ΔEs^k	$P_{Es}\%^l$
1a1	0.15	37.0	0.18	37.6	0.35	33.4	0.11	41.6	0.15	36.4	0.12	32.4
1a1′	4.22	0.0	4.43	0.0	4.94	0.0	4.77	0.0	4.31	0.0	1.66	2.4
1a1″	4.69	0.0	4.56	0.0	4.36	0.0	5.17	0.0	4.96	0.0	2.43	0.7
1a2	0.93	9.9	1.20	6.8	1.67	3.6	1.33	5.3	0.89	10.6	0.72	11.9
1b1	0.00	47.5	0.0	51.3	0.00	60.0	0.00	50.1	0.00	47.2	0.00	40.0
1b1′	3.98	0.1	4.18	0.0	4.74	0.0	4.53	0.0	4.05	0.1	1.45	3.4
1b1″	3.98	0.1	4.05	0.1	4.36	0.0	4.55	0.0	4.24	0.0	4.69	0.0
1b2	1.29	5.4	1.51	4.0	1.79	2.9	1.65	3.1	1.25	5.7	0.87	9.2

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy at the B3LYP/6-31G** level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at the B3LYP/6-31G** level in the gas phase. [g,h] Relative energy (kcal/mol) and conformational distribution in the gas phase at the B3LYP/6-311++G**//B3LYP/6-31G** level, respectively. [i,j] Relative energy (kcal/mol) and conformational distribution in the gas phase at the B3PW91/6-31G**//B3LYP/6-31G** level, respectively. [k,l] Relative energy (kcal/mol) and conformational distribution in MeOH solution at the B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model, respectively.

Table S7. Important Thermodynamic Parameters of Compound **2** (au).

species	in gas phase						in MeOH
	E	*E′=E+ZPE*	*H*	*G*	E_{lbs}	*Ew*	*Es*
2a1	-2822.597322	-2821.907993	-2821.856801	-2821.994221	-2823.354767	-2821.534986	-2822.650035
2a1′	-2822.5901781	-2821.900600	-2821.849679	-2821.985525	-2823.346718	-2821.527563	-2822.642871
2a1″	-2822.592248	-2821.902060	-2821.851561	-2821.984266	-2823.347147	-2821.528264	-2822.644814
2a2	-2822.595748	-2821.906129	-2821.855126	-2821.991469	-2823.351891	-2821.533379	-2822.648684
2b1	-2822.597261	-2821.907858	-2821.856697	-2821.994041	-2823.354784	-2821.534898	-2822.650214

2b1′	-2822.590776	-2821.901366	-2821.850394	-2821.986994	-2823.347458	-2821.528137	-2822.642946
2b1″	-2822.591799	-2821.902487	-2821.851411	-2821.988085	-2823.348230	-2821.529139	-2822.642599
2b2	-2822.595334	-2821.905743	-2821.854723	-2821.991125	-2823.351511	-2821.532948	-2822.648642

E, E′, *H, G*: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at the B3LYP/6-31G** level; E_{lbs}: single point energy in gas at the B3LYP/6-311++G**// B3LYP/6-31G** level; E_s: single point energy in methanol solution at the B3LYP-SCRF/6-31G**// B3LYP/6-31G** level with COSMO model.

Table S8. Conformational Analysis of Compound **2**.

species	in gas phase										in MeOH	
	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$	$\Delta E_{lbs}{}^g$	$P_{Elbs}\%^h$	$\Delta E_w{}^i$	$P_{Ew}\%^j$	ΔEs^k	$P_{Es}\%^l$
2a1	0.00	44.3	0.00	47.5	0.00	52.1	0.01	47.6	0.00	45.2	0.11	37.3
2a1′	4.48	0.0	4.64	0.0	5.46	0.0	5.06	0.0	4.66	0.0	4.61	0.0
2a1″	3.18	0.2	3.72	0.1	6.25	0.0	4.79	0.0	4.22	0.0	3.39	0.2
2a2	0.99	8.4	1.17	6.6	1.73	2.8	1.82	2.3	1.01	8.2	0.96	8.9
2b1	0.04	41.5	0.08	41.2	0.11	43.0	0.00	48.5	0.06	41.2	0.00	45.1
2b1′	4.11	0.0	4.16	0.0	4.54	0.0	4.60	0.0	4.30	0.0	4.56	0.0
2b1″	3.47	0.1	3.46	0.1	3.85	0.1	4.11	0.0	3.67	0.1	4.78	0.0
2b2	1.25	5.4	1.41	4.4	1.94	2.0	2.05	1.5	1.28	5.2	0.99	8.5

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy at the B3LYP/6-31G** level in the gas phase, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at the B3LYP/6-31G** level in the gas phase. [g,h] Relative energy (kcal/mol) and conformational distribution at the B3LYP/6-311++G**//B3LYP/6-31G** level, respectively. [i,j] Relative energy (kcal/mol) and conformational distribution in the gas phase at the B3PW91/6-31G**//B3LYP/ 6-31G** level, respectively. [k,l] Relative energy (kcal/mol) and conformational distribution in MeOH solution at the B3LYP-SCRF/6-31G**//B3LYP/6-31G** level with COSMO model, respectively.

Table S9: Important Thermodynamic Parameters of Compound **3** in the Gas Phase (au).

species	*E*	*E′=E+ZPE*	*H*	*G*
3a1	-2822.586948	-2821.897946	-2821.846640	-2821.983991
3b1	-2822.587197	-2821.898049	-2821.846787	-2821.984185

E, E′, H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at the B3LYP/6-31G** level.

Table S10. Conformational Analysis of Compound **3** in the Gas Phase.

species	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$
3a1	0.16	43.4	0.06	47.3	0.12	44.9
3b1	0.00	56.5	0.00	52.7	0.00	55.1

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy, respectively (kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at the B3LYP/6-31G** level in the gas phase, respectively.

Table S11: Important Thermodynamic Parameters of Compound **4** in the Gas Phase (au).

species	*E*	*E′=E+ZPE*	*H*	*G*
4a1	-2822.5903321	-2821.900973	-2821.849723	-2821.986822
4b1	-2822.5899219	-2821.900680	-2821.849350	-2821.986852

E, E′, H, G: total energy, total energy with zero point energy (ZPE), enthalpy and Gibbs free energy in the gas phase at the B3LYP/6-31G** level.

Table 12. Conformational Analysis of Compound **4** in the Gas Phase.

species	ΔE^a	$P_E\%^b$	$\Delta E'^c$	$P_{E'}\%^d$	ΔG^e	$P_G\%^f$
4a1	0.00	60.7	0.00	57.7	0.02	49.2
4b1	0.26	39.3	0.18	42.3	0.00	50.8

[a,c,e] Relative energy, relative energy with *ZPE*, and relative Gibbs free energy, respectively

(kcal/mol). [b,d,f] Conformational distribution calculated by using the respective parameters above at the B3LYP/6-31G** level in the gas phase, respectively.

Table S13. Frequencies of Compound **1** at the B3LYP/6-31G** Level in the Gas Phase (cm^{-1}).

species	frequencies
1a1	16 23 26 34 39 42 64 72 92 97 101 104 114 128 131 143 151 160 170 175 208 229 238 240 242 267 271 280 291 303 309 333 348 358 361 373 388 392 407 421 424 430 436 440 451 454 470 490 517 523 527 548 557 570 593 601 613 637 652 675 683 714 722 730 739 748 801 829 839 848 855 874 909 918 935 954 962 966 1001 1020 1026 1028 1030 1051 1058 1063 1064 1067 1072 1075 1076 1098 1104 1120 1128 1138 1139 1149 1158 1174 1177 1193 1201 1211 1212 1214 1235 1240 1257 1262 1275 1280 1299 1330 1332 1338 1346 1351 1356 1364 1378 1380 1380 1383 1402 1409 1419 1419 1427 1432 1440 1446 1452 1459 1463 1467 1476 1487 1489 1496 1504 1506 1514 1514 1519 1524 1563 1632 1634 1667 1673 1709 2975 2991 2999 3007 3017 3017 3023 3042 3046 3047 3063 3080 3101 3102 3105 3124 3151 3166 3170 3176 3200 3214 3225 3278 3792 3793 3796 3831
1a1′	13 22 23 29 38 53 66 76 93 104 108 121 130 136 146 149 153 166 181 198 218 231 235 242 248 268 275 284 294 303 309 343 345 354 362 380 389 395 415 425 425 432 435 439 446 467 474 489 510 521 524 547 557 573 589 602 613 638 648 656 681 705 717 735 740 770 799 824 830 847 859 873 913 917 937 954 961 966 989 1014 1023 1027 1030 1054 1057 1061 1063 1069 1073 1075 1079 1092 1096 1120 1123 1138 1138 1140 1157 1172 1177 1188 1201 1209 1212 1213 1234 1239 1255 1260 1271 1279 1299 1324 1329 1337 1343 1355 1358 1371 1373 1378 1380 1383 1403 1408 1417 1421 1427 1432 1437 1446 1452 1457 1458 1466 1472 1484 1489 1501 1505 1507 1514 1516 1519 1520 1563 1628 1633 1665 1673 1708 2976 2995 3006 3017 3019 3021 3032 3044 3048 3055 3062 3079 3094 3098 3107 3124 3151 3170 3176 3185 3200 3214 3226 3277 3789 3791 3795 3833
1a1″	17 17 21 31 39 45 61 69 86 95 97 99 112 115 131 145 158 160 174 182 214 230 239 242 248 266 273 280 297 299 312 325 346 350 366 375 384 391 413 416 423 428 434 437 438 465 479 489 505 522 525 544 555 570 591 603 618 637 650 659 680 712 715 730 739 759 800 827 830 847 851 872 905 918 932 953 961 961 992 1016 1023 1029 1030 1045 1059 1066 1067 1068 1072 1074 1076 1089 1098 1120 1125 1138 1138 1144 1158 1173 1178 1192 1200 1209 1211 1218 1234 1238 1258 1264 1273 1279 1299 1326 1331 1338 1344 1352 1354 1370 1377 1377 1379 1382 1402 1408 1416 1420 1425 1428 1439 1443 1453 1459 1460 1466 1477 1485 1489 1495 1501 1505 1511 1518 1519 1526 1563 1626 1633 1665 1673 1707 2976 2989 3007 3009 3017 3023 3024 3035 3047 3063 3065 3080 3099 3116 3124 3124 3151 3163 3165 3176 3200 3214 3224 3272 3792 3797 3799 3831
1a2	16 21 25 31 42 46 67 73 90 99 103 117 133

	143 146 151 155 164 175 192 209 230 237 242 247 263 274 284 295 304 316 320 341 351 362 371 387 404 409 422 425 429 435 442 453 460 472 489 519 522 526 544 554 571 594 605 611 636 653 676 679 700 723 734 736 744 800 829 844 848 871 874 908 919 935 954 961 970 998 1022 1026 1027 1030 1058 1061 1065 1071 1073 1073 1075 1077 1097 1103 1118 1127 1138 1139 1145 1161 1171 1178 1199 1201 1211 1212 1218 1234 1238 1258 1261 1271 1278 1299 1322 1331 1337 1345 1353 1355 1367 1373 1376 1381 1383 1403 1409 1416 1424 1427 1431 1440 1449 1454 1458 1460 1466 1480 1489 1491 1505 1508 1512 1513 1519 1519 1524 1563 1630 1633 1669 1673 1704 2976 2996 3008 3015 3017 3022 3030 3037 3047 3052 3064 3079 3099 3110 3115 3123 3150 3165 3165 3176 3201 3213 3225 3236 3792 3792 3795 3832
1b1	16 19 24 32 37 44 66 78 84 89 99 104 115 133 135 142 152 163 166 179 216 231 236 241 243 265 274 282 295 301 309 327 335 355 363 378 388 397 409 422 424 430 435 439 454 457 470 488 519 523 528 546 556 568 593 600 614 637 652 675 688 710 718 730 738 747 800 829 841 848 854 873 908 917 933 953 962 968 1000 1021 1026 1028 1030 1050 1059 1063 1064 1068 1072 1074 1076 1097 1105 1119 1126 1137 1139 1149 1162 1172 1178 1193 1200 1211 1211 1214 1235 1238 1257 1262 1273 1278 1299 1329 1331 1337 1346 1353 1355 1364 1375 1377 1379 1382 1404 1408 1417 1418 1425 1433 1440 1446 1451 1460 1462 1466 1478 1485 1488 1496 1504 1511 1514 1514 1518 1522 1563 1631 1634 1667 1673 1708 2975 2992 3004 3008 3017 3018 3020 3042 3044 3048 3063 3079 3098 3103 3112 3124 3151 3165 3166 3176 3202 3214 3225 3277 3791 3792 3796 3833
1b1′	14 21 24 31 36 56 67 77 88 104 112 121 130 135 150 151 156 168 178 188 219 232 234 242 247 266 273 285 296 302 307 334 337 357 363 375 390 396 418 424 428 433 435 439 445 470 473 485 516 518 524 546 556 573 589 602 614 641 649 655 683 704 716 734 738 770 799 825 829 846 849 873 910 918 937 954 962 964 991 1014 1024 1028 1030 1055 1057 1060 1064 1069 1074 1076 1079 1092 1096 1120 1123 1138 1138 1142 1158 1172 1178 1187 1200 1209 1211 1214 1234 1238 1257 1261 1274 1278 1299 1325 1327 1337 1345 1355 1357 1372 1374 1376 1380 1383 1400 1408 1417 1420 1427 1430 1438 1446 1454 1456 1460 1465 1472 1486 1489 1499 1502 1505 1511 1512 1519 1524 1563 1626 1633 1666 1673 1709 2976 2995 3006 3017 3017 3023 3032 3042 3048 3054 3064 3079 3095 3098 3108 3126 3151 3168 3176 3183 3204 3214 3226 3290 3791 3793 3795 3832
1b1″	15 20 22 33 37 52 63 77 87 99 106 114 120 131 145 151 155 169 172 182 222 230 238 243 244 264 273 286 296 298 312 328 340 347 366 379 388 393 417 420 424 431 434 438 439 467 479 486 511 523 523 546 553 566 591 604 614 640 651 660 681 711 717 732 739 761 799 828 832 846 861 872 903 918 933 954 961 967 989 1014 1024 1030 1031 1046 1059 1066 1067 1068 1074 1074 1076 1090 1098 1120 1125 1138 1138 1145 1161 1173 1178 1192 1201 1209 1211 1217 1233 1238 1257 1268 1274 1279 1298

	1327 1330 1338 1342 1351 1354 1371 1375 1379 1379 1381 1404 1409 1417 1422 1424 1427 1439 1443 1451 1459 1461 1466 1476 1488 1490 1496 1500 1504 1510 1514 1518 1528 1562 1628 1633 1667 1673 1707 2975 2988 3007 3012 3016 3024 3026 3034 3047 3063 3065 3079 3099 3112 3125 3127 3151 3160 3168 3176 3203 3213 3225 3255 3790 3796 3798 3830
1b2	16 20 22 31 39 47 69 73 87 100 105 116 131 133 149 152 156 159 178 194 217 223 236 241 247 263 273 280 294 303 317 322 341 351 367 375 385 400 408 421 424 429 434 441 450 461 471 489 513 523 527 542 554 573 593 599 617 636 653 675 686 693 718 734 739 746 802 828 841 848 851 874 907 919 936 952 961 962 1006 1021 1025 1026 1030 1058 1062 1064 1072 1073 1074 1075 1076 1097 1104 1118 1127 1137 1139 1145 1156 1174 1178 1198 1201 1211 1211 1218 1234 1238 1258 1260 1273 1278 1299 1324 1330 1338 1350 1353 1356 1368 1373 1377 1379 1381 1401 1408 1418 1423 1427 1431 1440 1447 1451 1459 1461 1467 1478 1487 1489 1504 1506 1509 1513 1519 1520 1528 1563 1629 1633 1667 1673 1706 2976 2994 3008 3014 3017 3021 3027 3034 3047 3053 3063 3079 3099 3112 3115 3124 3151 3165 3165 3176 3200 3214 3226 3266 3791 3793 3796 3832

Table S14. Frequencies of Compound **2** at the B3LYP/6-31G** Level in the Gas Phase (cm^{-1}).

species	frequencies
2a1	6. 9. 16. 20. 23. 36. 38. 43. 46. 61. 69. 77. 79. 82. 87. 91. 101. 103. 116. 119. 128. 145. 148. 150. 154. 158. 163. 176. 180. 181. 196. 196. 202. 213. 228. 235. 238. 243. 256. 259. 272. 275. 289. 294. 296. 297. 302. 309. 320. 321. 326. 329. 338. 348. 356. 357. 360. 362. 368. 378. 386. 390. 405. 416. 420. 424. 433. 434. 436. 446. 457. 470. 474. 481. 489. 489. 499. 518. 522. 525. 538. 541. 550. 555. 557. 563. 568. 579. 593. 601. 605. 614. 625. 633. 637. 652. 656. 673. 680. 681. 684. 685. 703. 719. 728. 739. 744. 747. 752. 770. 787. 801. 805. 829. 838. 839. 842. 847. 855. 864. 874. 886. 917. 918. 937. 954. 961. 966. 972. 996. 1001. 1017. 1020. 1025. 1030. 1039. 1058. 1060. 1062. 1065. 1068. 1074. 1075. 1091. 1102. 1105. 1117. 1127. 1138. 1146. 1155. 1158. 1162. 1168. 1176. 1178. 1179. 1193. 1200. 1201. 1211. 1213. 1216. 1220. 1224. 1239. 1247. 1249. 1255. 1278. 1278. 1295. 1299. 1308. 1324. 1329. 1330. 1331. 1338. 1340. 1345. 1350. 1356. 1360. 1367. 1380. 1381. 1384. 1388. 1391. 1396. 1404. 1405. 1407. 1416. 1421. 1422. 1427. 1433. 1442. 1454. 1459. 1464. 1467. 1476. 1487. 1489. 1493. 1496. 1501. 1505. 1505. 1516. 1517. 1519. 1525. 1555. 1556. 1563. 1632. 1634. 1646. 1655. 1667. 1670. 1673. 1678. 1708. 1776. 1823. 2987. 2993. 3002. 3005. 3017. 3029. 3042. 3047. 3050. 3079. 3098. 3099. 3103. 3113. 3124. 3151. 3165. 3167. 3176. 3185. 3201. 3204. 3214. 3226. 3226. 3280. 3627. 3705. 3744. 3761. 3772. 3779. 3793. 3839.
2a1′	7 10 13 21 31 33 40 45 56 58 71 78 83 93 95 102 107 120 121 128 137 146 149 152 153 166 168

	174 180 182 195 198 203 222 229 235 240 244 253 260 272 280 288 295 297 297 304 310 320 323 328 331 345 349 353 358 362 365 370 379 384 388 408 419 424 426 431 434 435 451 461 469 482 487 488 490 505 512 522 523 538 541 549 556 558 561 567 580 593 599 605 614 625 634 639 648 653 658 680 681 684 685 702 714 733 739 744 749 761 773 789 799 805 825 829 839 843 846 855 863 872 888 916 918 939 954 960 966 976 987 1000 1011 1021 1024 1030 1042 1055 1061 1061 1067 1072 1075 1077 1083 1090 1100 1114 1130 1137 1141 1147 1158 1161 1167 1176 1178 1179 1190 1200 1200 1210 1211 1215 1222 1225 1238 1248 1251 1254 1278 1278 1293 1299 1307 1324 1328 1329 1331 1334 1337 1344 1350 1355 1363 1377 1379 1380 1385 1389 1392 1394 1400 1404 1407 1414 1419 1422 1426 1434 1443 1452 1460 1461 1466 1472 1483 1489 1494 1500 1502 1504 1507 1511 1516 1519 1519 1555 1557 1563 1628 1633 1646 1655 1666 1671 1673 1678 1706 1777 1823 2990 2999 3006 3016 3018 3032 3043 3047 3055 3080 3094 3098 3108 3112 3123 3152 3163 3169 3173 3183 3203 3204 3213 3225 3225 3283 3628 3709 3744 3760 3772 3779 3792 3841
2a1″	11 17 23 28 35 40 43 50 57 63 73 79 82 86 90 97 98 117 121 125 141 147 154 156 158 167 175 181 190 196 199 210 222 233 238 241 250 255 259 270 282 287 297 298 299 303 308 311 323 326 329 338 350 351 352 359 363 364 379 383 385 390 409 419 424 428 433 438 439 452 462 468 480 488 491 497 505 510 522 524 540 541 551 556 559 560 573 581 595 603 606 617 625 634 636 647 653 658 680 681 684 686 704 716 732 739 745 751 765 773 789 802 806 823 833 841 843 846 848 865 875 889 913 919 936 950 963 964 971 988 996 1011 1020 1024 1029 1038 1057 1059 1061 1064 1070 1071 1075 1081 1089 1098 1110 1127 1136 1143 1147 1158 1159 1169 1169 1176 1177 1186 1200 1201 1209 1210 1214 1223 1225 1242 1247 1254 1262 1276 1277 1291 1302 1305 1321 1328 1329 1329 1335 1337 1343 1350 1354 1362 1372 1377 1380 1384 1386 1391 1393 1396 1403 1409 1413 1418 1421 1427 1438 1442 1451 1459 1463 1465 1469 1484 1488 1491 1494 1498 1501 1505 1506 1515 1517 1519 1554 1556 1563 1625 1631 1645 1652 1665 1669 1670 1677 1708 1775 1821 2987 3001 3003 3021 3031 3040 3048 3058 3060 3085 3099 3112 3113 3114 3121 3156 3164 3178 3180 3190 3201 3208 3213 3225 3226 3309 3628 3702 3744 3761 3771 3781 3790 3790
2a2	8 12 12 20 28 32 42 45 54 56 71 78 80 85 91 101 105 115 121 133 140 145 149 151 156 160 161 174 179 186 194 200 210 217 224 235 240 245 257 261 274 280 286 295 296 296 303 313 319 321 324 329 336 348 350 357 361 366 368 372 383 390 408 418 424 425 430 434 437 446 464 470 479 483 487 489 497 520 522 524 538 539 549 554 557 559 571 579 592 603 608 614 625 632 637 653 656 675 677 680 685 685 699 709 733 736 742 744 751 770 788 800 805 829 836 842 844 848 864 869 874 886 916 919 937 955 962 968 974 998 999 1020 1021 1025 1031 1043 1060 1064 1069 1071

	1073 1077 1077 1087 1098 1101 1120 1126 1138 1144 1152 1158 1162 1169 1173 1178 1178 1197 1200 1202 1211 1214 1218 1220 1224 1238 1247 1248 1255 1278 1280 1295 1299 1308 1324 1328 1329 1332 1335 1337 1345 1350 1355 1361 1372 1380 1381 1382 1388 1392 1394 1400 1404 1409 1416 1421 1423 1428 1432 1442 1452 1459 1462 1466 1478 1488 1490 1493 1499 1504 1508 1513 1515 1519 1520 1523 1555 1557 1563 1630 1634 1646 1655 1668 1670 1673 1678 1703 1776 1823 2992 3001 3007 3016 3016 3030 3036 3047 3051 3079 3099 3110 3112 3117 3123 3150 3164 3165 3167 3176 3202 3204 3213 3225 3226 3237 3627 3702 3744 3761 3773 3780 3793 3840
2b1	7 8 13 23 26 35 40 44 46 62 70 74 80 81 85 88 99 105 118 120 131 143 147 153 156 163 170 177 180 185 195 196 201 219 225 232 238 246 255 258 274 279 291 293 296 297 303 309 319 320 325 328 331 345 354 358 361 365 367 379 384 391 408 417 421 425 432 432 436 445 460 471 476 480 485 487 497 520 522 526 538 539 550 555 556 561 568 579 593 601 605 616 623 632 637 651 656 673 680 683 685 687 704 713 727 739 744 747 752 770 787 800 805 829 838 842 843 848 861 863 873 887 916 918 936 955 962 967 972 995 999 1019 1020 1025 1031 1038 1059 1060 1062 1068 1071 1073 1076 1091 1102 1105 1117 1127 1138 1147 1153 1158 1162 1169 1174 1178 1179 1193 1199 1201 1211 1213 1216 1221 1225 1237 1247 1249 1254 1278 1279 1295 1299 1309 1324 1327 1330 1332 1337 1343 1344 1350 1355 1362 1370 1380 1381 1382 1388 1391 1394 1403 1406 1408 1415 1421 1422 1427 1433 1443 1456 1459 1465 1467 1480 1487 1489 1494 1498 1505 1505 1514 1515 1516 1518 1519 1555 1557 1563 1632 1634 1646 1655 1668 1671 1673 1678 1706 1775 1822 2988 2995 3008 3009 3016 3031 3041 3047 3061 3078 3097 3104 3111 3117 3124 3150 3163 3163 3164 3177 3201 3204 3214 3225 3226 3263 3629 3704 3745 3761 3774 3780 3792 3840
2b1′	6 6 15 21 29 33 36 45 56 61 71 78 84 86 93 100 109 119 123 130 144 146 149 151 157 163 167 172 180 180 195 197 204 224 230 235 241 244 252 259 270 279 289 295 296 297 305 306 320 323 328 331 337 348 355 357 361 362 366 375 383 389 410 418 424 426 430 435 436 450 464 470 484 485 486 491 505 516 520 523 538 539 548 556 557 561 567 580 593 599 605 614 623 633 640 647 654 657 680 681 684 685 701 713 733 738 744 749 762 773 789 799 805 824 830 839 843 846 849 864 873 888 916 918 938 954 962 964 976 990 999 1012 1021 1024 1030 1042 1056 1059 1060 1066 1072 1075 1075 1082 1088 1099 1113 1130 1138 1138 1147 1158 1162 1167 1175 1177 1180 1188 1200 1201 1210 1211 1215 1219 1224 1238 1248 1251 1254 1278 1279 1293 1298 1306 1324 1327 1328 1329 1335 1338 1346 1350 1355 1361 1375 1377 1380 1383 1388 1392 1396 1399 1403 1407 1413 1418 1420 1425 1432 1440 1451 1460 1461 1465 1471 1485 1488 1494 1495 1499 1503 1503 1507 1515 1518 1523 1555 1557 1563 1626 1633 1646 1655 1666 1671 1673 1678 1706 1776 1823 2991 3004 3005 3016 3020 3033 3042 3046 3055 3079 3095 3099 3108 3112 3124 3151 3163 3169 3176 3188 3205 3205 3214 3225 3226 3295 3626 3705 3744 3761

	3774 3780 3793 3838
2b1″	5 11 14 25 27 35 42 43 47 66 70 77 84 84 89 97 106 116 118 120 125 130 146 150 154 162 166 172 179 180 193 197 209 225 232 234 241 246 257 258 276 285 289 295 296 297 304 307 319 320 325 328 335 341 348 358 363 366 369 379 383 389 413 420 421 424 431 435 436 449 464 471 480 483 489 490 506 514 522 524 534 538 549 553 557 560 571 578 596 599 605 617 623 633 639 649 656 658 679 680 683 685 703 714 730 738 744 750 760 771 788 799 805 830 832 837 843 847 861 864 872 887 916 920 936 956 962 966 971 986 997 1011 1019 1025 1031 1038 1059 1061 1062 1067 1070 1074 1076 1083 1093 1101 1115 1129 1138 1146 1151 1158 1162 1167 1176 1178 1180 1193 1200 1201 1211 1212 1214 1222 1224 1238 1248 1254 1256 1278 1280 1293 1298 1307 1324 1327 1328 1331 1336 1339 1344 1350 1354 1360 1373 1379 1380 1382 1388 1392 1393 1400 1402 1407 1414 1419 1421 1425 1433 1439 1451 1460 1463 1466 1476 1488 1490 1494 1494 1501 1501 1505 1511 1515 1519 1526 1555 1557 1563 1628 1633 1646 1654 1668 1671 1673 1678 1705 1774 1822 2985 3001 3005 3010 3017 3030 3047 3048 3063 3079 3099 3112 3115 3123 3124 3150 3162 3164 3174 3175 3204 3205 3213 3225 3226 3248 3629 3696 3744 3761 3772 3780 3791 3838
2b2	8 9 16 20 28 30 37 45 55 58 71 79 81 85 92 102 105 118 121 126 138 142 150 153 156 161 163 170 179 186 193 198 215 221 228 232 240 247 257 261 273 278 283 294 296 296 302 313 320 323 325 329 333 344 347 357 361 366 367 376 384 391 405 417 424 425 431 432 437 446 467 471 481 484 486 490 494 517 522 526 535 538 550 554 557 559 574 580 592 604 607 616 625 632 638 651 656 674 680 682 685 688 693 704 734 738 744 745 751 769 788 802 805 829 838 840 843 847 853 864 874 887 916 920 937 953 961 962 973 998 1005 1019 1021 1024 1030 1043 1061 1064 1070 1071 1073 1074 1076 1087 1097 1102 1120 1126 1138 1143 1151 1157 1161 1169 1176 1178 1179 1198 1200 1202 1211 1215 1217 1220 1224 1239 1247 1249 1255 1279 1279 1294 1299 1307 1324 1327 1328 1330 1335 1339 1349 1350 1355 1361 1372 1379 1381 1382 1389 1392 1395 1398 1405 1408 1416 1421 1423 1426 1433 1441 1452 1460 1462 1466 1478 1487 1488 1494 1499 1504 1506 1509 1516 1519 1520 1528 1555 1557 1563 1629 1633 1646 1655 1667 1671 1673 1678 1706 1776 1823 2989 3001 3008 3016 3017 3029 3033 3048 3053 3079 3099 3111 3113 3116 3125 3151 3163 3164 3165 3177 3200 3205 3213 3224 3226 3265 3626 3703 3743 3761 3773 3780 3792 3840

Table S15. Frequencies of Compound **3** at the B3LYP/6-31G** Level in the Gas Phase (cm^{-1}).

species	frequencies
3a1	6. 9. 16. 22. 29. 31. 39. 44. 50. 57. 76. 82. 85.

	88. 90. 94. 96. 102. 111. 114. 123. 141. 146. 149. 150. 157. 163. 174. 180. 182. 187. 194. 208. 213. 226. 235. 241. 244. 257. 262. 269. 271. 290. 293. 294. 297. 304. 307. 312. 321. 328. 333. 336. 346. 352. 353. 357. 362. 362. 369. 380. 389. 390. 405. 420. 424. 425. 429. 436. 443. 452. 468. 478. 480. 490. 493. 500. 510. 519. 523. 534. 542. 551. 554. 556. 561. 572. 575. 592. 597. 606. 616. 624. 635. 639. 643. 652. 656. 678. 681. 687. 687. 696. 718. 730. 739. 740. 746. 750. 783. 791. 801. 807. 829. 835. 839. 841. 847. 854. 867. 874. 878. 917. 920. 934. 954. 962. 966. 972. 994. 1005. 1021. 1025. 1030. 1043. 1048. 1057. 1058. 1059. 1063. 1068. 1074. 1075. 1079. 1099. 1102. 1105. 1124. 1138. 1141. 1145. 1156. 1158. 1165. 1175. 1177. 1180. 1194. 1199. 1200. 1210. 1210. 1214. 1225. 1229. 1235. 1239. 1248. 1250. 1274. 1279. 1285. 1294. 1299. 1321. 1327. 1329. 1337. 1338. 1338. 1344. 1345. 1355. 1358. 1360. 1374. 1380. 1382. 1383. 1388. 1393. 1397. 1404. 1407. 1412. 1418. 1420. 1427. 1436. 1442. 1451. 1459. 1461. 1466. 1475. 1485. 1486. 1488. 1496. 1504. 1504. 1504. 1508. 1517. 1518. 1523. 1554. 1557. 1563. 1632. 1634. 1647. 1658. 1667. 1671. 1673. 1681. 1708. 1795. 1827. 2965. 3005. 3009. 3017. 3042. 3048. 3049. 3052. 3065. 3080. 3093. 3102. 3103. 3108. 3125. 3151. 3155. 3168. 3175. 3182. 3202. 3205. 3213. 3225. 3237. 3283. 3604. 3729. 3754. 3769. 3780. 3782. 3795. 3840.
3b1	7 9 12 22 29 33 38 45 51 58 76 81 84 86 88 90 95 101 109 115 129 143 147 151 153 163 166 171 180 182 188 194 208 219 232 233 242 247 257 261 269 278 291 294 295 297 304 306 311 323 327 330 337 342 347 353 360 362 366 371 381 387 391 402 419 424 425 433 435 440 449 471 473 482 488 496 504 513 519 523 534 542 552 555 558 561 573 576 590 597 606 615 624 634 641 647 652 658 677 681 688 691 698 712 728 738 741 746 750 782 790 799 807 829 836 841 844 849 860 867 872 878 918 921 933 954 962 967 973 992 1003 1023 1025 1030 1041 1047 1055 1060 1060 1068 1070 1073 1075 1079 1099 1103 1105 1126 1139 1142 1146 1156 1159 1165 1173 1177 1181 1193 1200 1201 1210 1211 1214 1226 1229 1236 1238 1249 1251 1274 1278 1284 1292 1299 1322 1329 1330 1337 1338 1339 1343 1345 1354 1358 1360 1375 1380 1381 1382 1389 1394 1397 1407 1409 1412 1418 1419 1425 1436 1441 1453 1458 1459 1466 1480 1486 1487 1488 1502 1504 1504 1509 1512 1514 1519 1520 1555 1557 1563 1632 1634 1647 1658 1668 1671 1673 1681 1706 1794 1826 2964 3007 3017 3023 3040 3047 3049 3061 3065 3079 3091 3105 3110 3117 3124 3151 3154 3161 3166 3176 3202 3205 3214 3223 3237 3261 3605 3728 3755 3769 3780 3782 3795 3840

Table S16. Frequencies of Compound **4** at the B3LYP/6-31G** Level in the Gas Phase (cm^{-1}).

species	frequencies
4a1	7 10 12 21 30 31 40 45 52 60 75 81 82

	88 88 91 98 103 108 117 130 142 147 150 151 164 167 171 180 184 187 195 207 219 227 235 239 241 256 259 268 278 292 294 295 297 307 308 314 324 329 333 337 341 352 361 361 364 370 376 382 390 394 411 416 420 424 428 429 436 445 456 470 483 490 493 502 510 520 523 535 542 552 554 555 558 571 575 592 597 606 613 624 633 639 645 652 657 677 681 687 689 696 712 734 739 740 745 750 784 791 800 806 829 834 840 842 848 864 868 873 886 918 920 935 955 961 967 972 997 1016 1020 1025 1030 1043 1047 1057 1060 1064 1068 1072 1073 1075 1079 1096 1100 1113 1125 1132 1136 1139 1154 1163 1168 1172 1177 1180 1191 1200 1201 1208 1211 1213 1215 1228 1238 1247 1250 1253 1274 1279 1285 1296 1299 1316 1321 1328 1329 1337 1343 1344 1348 1356 1359 1368 1376 1380 1382 1384 1388 1393 1397 1407 1410 1414 1417 1424 1427 1435 1438 1444 1458 1459 1466 1480 1485 1487 1489 1504 1506 1508 1509 1509 1513 1518 1520 1555 1556 1562 1632 1634 1647 1658 1667 1670 1673 1681 1708 1791 1828 3006 3016 3017 3025 3039 3047 3048 3048 3063 3080 3086 3093 3105 3124 3125 3152 3155 3164 3168 3175 3203 3204 3214 3226 3236 3255 3608 3731 3755 3782 3795 3798 3815 3840
4b1	7 9 16 22 27 32 37 44 51 59 68 76 80 85 90 94 96 103 110 115 131 140 148 151 153 161 163 174 179 183 186 194 208 222 224 232 241 244 256 259 268 273 292 294 295 298 305 307 314 323 327 330 335 341 351 359 361 365 369 379 381 390 394 412 416 420 424 428 433 437 444 452 470 483 487 492 500 507 518 524 535 541 551 554 555 559 569 575 592 596 606 612 623 631 640 642 651 658 676 682 687 692 695 709 735 739 740 746 752 784 792 801 806 830 833 838 840 848 856 868 874 886 917 920 934 954 962 966 972 1000 1016 1019 1024 1029 1043 1048 1057 1058 1061 1066 1072 1073 1075 1079 1097 1100 1112 1123 1132 1136 1140 1154 1164 1166 1176 1178 1180 1190 1200 1201 1208 1211 1212 1215 1228 1238 1247 1250 1253 1273 1278 1285 1296 1300 1315 1321 1328 1329 1338 1344 1345 1351 1356 1357 1368 1376 1379 1382 1384 1388 1393 1398 1406 1410 1413 1417 1425 1429 1437 1438 1447 1460 1460 1466 1474 1485 1488 1489 1500 1504 1505 1506 1508 1510 1518 1523 1555 1556 1563 1632 1635 1647 1659 1666 1671 1673 1681 1710 1791 1829 3009 3009 3017 3024 3037 3045 3047 3049 3063 3080 3087 3093 3106 3109 3125 3152 3155 3164 3176 3185 3201 3203 3214 3227 3236 3282 3609 3730 3755 3782 3796 3797 3817 3840

Table S17. Key Transitions and Their Related Rotatory and Oscillator Strengths of **1** at the B3LYP-SCRF//B3LYP/6-31G** Level with COSMO Model in MeOH.

species	transition	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
	126→127	3.46	358	0.076	11.1	11.8

	125→127	3.80	326	0.022	-21.4	-22.3
	124→127	4.54	273	0.304	-21.6	-19.5
	126v128	5.06	245	0.025	16.3	15.6
1b1	126→127	3.47	357	0.080	7.0	5.8
	125→127	3.78	328	0.020	-18.0	-19.3
	124→127	4.53	273	0.301	-21.1	-23.3
	125→128	5.07	245	0.033	7.6	6.9

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).

Table S18. Key Transitions and Their Related Rotatory and Oscillator Strengths of L-**1a1** at the B3LYP/6-31G** Level in the Gas Phase.

species	transition	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
L-**1a1**	126→127	3.51	353	0.068	10.3	11.7
	125→127	3.88	320	0.019	-21.2	-23.0
	122→127	4.22	294	0.006	6.2	5.4
	124→127	4.61	269	0.233	-32.5	-30.6
	126→129	5.20	239	0.018	9.0	8.4
	120→127	5.22	237	0.001	-1.6	-2.0

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).

Table S19. Key Transitions and Their Related Rotatory and Oscillator Strengths of **2b1** at the B3LYP/6-31G** Level in the Gas Phase.

transition	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
203→204	3.49	355	0.066	1.2	-4.1
202→205	3.85	322	0.045	-9.0	-15.1
201→204	3.93	315	0.012	-17.4	-19.2
202→206	4.24	293	0.072	-42.5	-47.0

199→204	4.58	271	0.273	-48.2	-53.5
197→205	4.67	266	0.020	-17.3	-18.7
198→206	4.98	249	0.037	-4.1	-12.4
202→208	4.99	248	0.088	48.4	49.7
197→206	5.10	243	0.040	50.7	54.3
191→205	5.22	237	0.011	-13.6	-16.3
200→208	5.31	234	0.143	4.0	18.8

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).

Table S20. Key Transitions, Oscillator Strengths, and Rotatory Strengths of Conformer **3a1** of compound **3** at the B3LYP/6-31G** Level in the Gas Phase.

excited state	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
203→204	3.47	357	0.062	10.8	13.9
200→204	3.92	316	0.012	-21.8	-23.5
202→206	4.16	298	0.064	4.9	1.1
201→205	4.33	286	0.058	25.3	26.2
201→206	4.49	276	0.115	-38.6	-42.4
199→204	4.57	271	0.004	2.1	2.3
198→204	4.60	270	0.244	32.2	36.5
199→205	4.66	266	0.043	22.9	26.7
199→206	4.83	257	0.091	17.5	14.5
197→206	5.01	247	0.062	-134.1	-144.6
200→207	5.12	242	0.021	1.4	-4.3
201→208	5.29	234	0.014	21.5	26.2

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).

Table S21. Key Transitions, Oscillator Strengths, and Rotatory Strengths of Compound **4** at the B3LYP/6-31G** Level in the Gas Phase.

species	excited state	ΔE^a (eV)	λ^b (nm)	f^c	$R_{vel}{}^d$	$R_{len}{}^e$
	202→204	3.5069	353.54	0.0668	13.9304	18.7242
	200→204	3.8688	320.47	0.0154	-23.0954	-24.2140
	203→206	4.1666	297.57	0.0569	-12.3109	-15.8354
	201→205	4.3093	287.71	0.0657	-34.9020	-38.3278
	201→206	4.4947	275.85	0.1024	28.0704	31.8707
4a1	198→204	4.5960	269.77	0.2553	-114.2482	-115.9900
	199→205	4.6789	264.98	0.0451	-27.0822	-29.2683
	199→205	4.8306	256.66	0.0958	-13.7940	-11.5774
	203→209	5.0076	247.59	0.1089	171.1894	180.8287
	197→206	5.0555	245.25	0.0655	-38.8400	-45.4286
	198→205	5.3297	232.63	0.0874	-17.0730	-19.2904
	202→204	3.4982	354.42	0.0622	9.5191	5.6905
	200→204	3.8901	318.71	0.0148	-15.3622	-17.1611
	203→206	4.1735	297.07	0.0589	-6.3313	-11.2453
	201→205	4.3161	287.26	0.0641	-21.7037	-23.8069
	201→206	4.4959	275.77	0.0979	33.6459	37.1557
4b1	198→204	4.6074	269.10	0.2403	-89.0553	-94.6709
	199→205	4.6873	264.51	0.0441	-29.0002	-32.6137
	199→205	4.8392	256.21	0.0910	-11.2914	-7.1404
	203→209	5.0079	247.58	0.1187	172.7144	181.2018
	197→206	5.0611	244.98	0.0553	-44.3572	-49.7353
	201→209	5.2814	234.76	0.0090	9.7549	12.3116

[a] Excitation energy. [b] Wavelength. [c] Oscillator strength. [d] Rotatory strength in velocity form (10^{-40} cgs). [e] Rotatory strength in length form (10^{-40} cgs).