

# Electronic Supplementary Information

## Synthesis of pendant fullerene dimers by aminomethylation reaction of fulleropyrrolidines bearing ketone moieties

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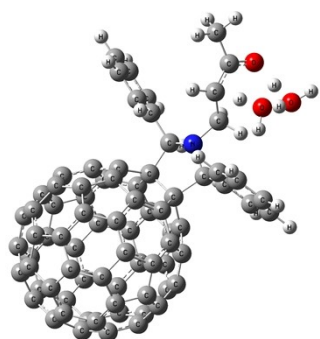
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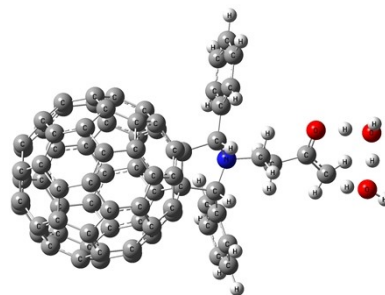
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## Computational results for mechanistic study

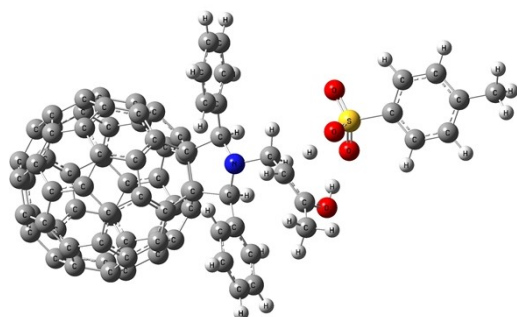
Fig. S1 Optimized transition-state geometries of different reaction pathways



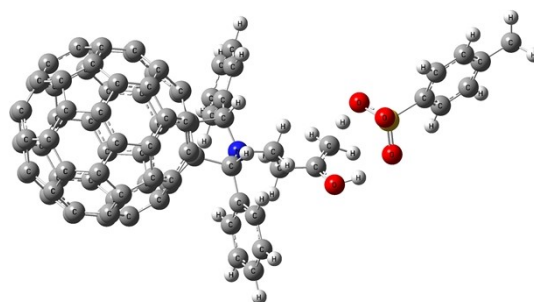
**Ts1a-H<sub>2</sub>O**



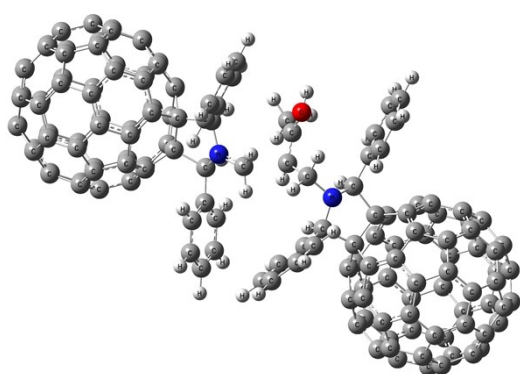
**Ts1b-H<sub>2</sub>O**



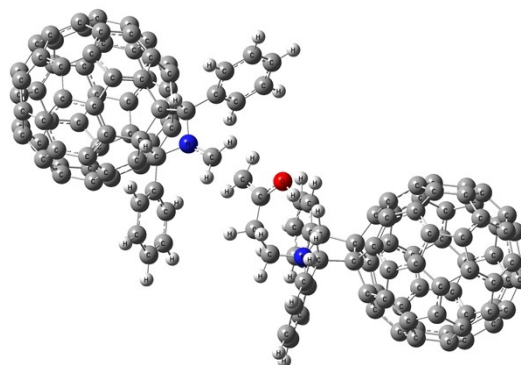
**Ts1a-TsOH**



**Ts1b-TsOH**



**Ts2a**



**Ts2b**

**Table S1** Total energy (E) and relative energy ( $\Delta E$ ), solvation effect, entropy (S), relative entropy ( $\Delta S$ ) and entropic contributions to free energy at 313.15 K (TS) for keto–enol tautomerism catalyzed by TsOH and H<sub>2</sub>O.

	In chlorobenzene		In gas phase		Solvation effect (kcal/mol)	S cal/(mol·K)	ΔS cal/(mol·K)	TS (kcal/mol) T = 313.15 K
	E (a.u)	ΔE (kcal/mol)	E (a.u)	ΔE (kcal/mol)				
<b>1</b>	- 3113.211 584		- 3113.1 32237			232.80 8		
H <sub>2</sub> O	- 76.42699 78		- 76.420 707			45.136		
TsOH	- 895.3080 111		- 895.28 93948			107.40 1		
TsO <sup>-</sup>	- 894.8550 085		- 894.77 55879			102.82 3		
TS1a-TsOH	- 4008.506 634	8.1	- 4008.4 14118	4.7	3.4	288.29 9	-51.9	-16.3
TS1b-TsOH	- 4008.502 958	10.4	- 4008.4 09109	7.9	2.5	291.06 8	-49.1	-15.4
TS1a-H <sub>2</sub> O	- 3266.031 607	21.3	- 3265.9 51335	14.0	7.3	242.71 6	-80.4	-25.2
TS1b-H <sub>2</sub> O	- 3266.029 133	22.9	- 3265.9 47625	16.3 S5	6.6	245.35 9	-77.7	-24.3

**Table S2** Calculated thermal corrections to Gibbs free energies ( $TCG$ ), electronic energies ( $E$ ) in solvent, Gibbs free energies ( $G$ ), relative Gibbs free energies ( $\Delta G$  relative to reactants **1a** and **E1**), and imaginary frequencies only for transition states

Species	$TCG(\text{a.u.})^a$ (1)	$E(\text{a.u.})^b$ (2)	$G(\text{a.u.})$ (3)=(1)+(2)	$\Delta G$ (kcal/mol)	Imaginary frequency ( $\text{cm}^{-1}$ )
<b>1a</b>	0.630198	- 3113.21158 4	-3112.581386		
<b>E1</b>	0.56531	- 2920.47681 1	-2919.911501		
<b>H<sub>2</sub>O</b>	0.002417	- 76.4269978	-76.4245808		
<b>TsOH</b>	0.100529	- 895.308011 1	-895.2074821		
<b>TsO<sup>-</sup></b>	0.090541	- 894.855008 5	-894.7644675		
<b>TS1a-H<sub>2</sub>O</b>	0.671294	- 3266.03160 7	-3265.360313	44.1	1491.283 6i
<b>TS1b-H<sub>2</sub>O</b>	0.669277	- 3266.02913 3	-3265.359856	44.4	1678.384 5i

<b>TS1a-TsOH</b>	0.753496	- 4008.50663 4	-4007.753138	22.4	1150.575 9i
<b>TS1b-TsOH</b>	0.75274	- 4008.50295 8	-4007.750218	24.3	1142.496 6i
<b>G1</b>	0.63576	- 3113.19871 9	-3112.562959	11.6	
<b>I1</b>	0.637798	- 3113.19567 8	-3112.55788	14.8	
<b>TS2a</b>	1.223432	- 6033.67981	-6032.456378	22.9	
<b>TS2b</b>	1.221825	- 6033.66352 2	-6032.441697	32.1	207.3654 i
<b>3aa</b>	1.21366	- 6033.29959 3	-6032.085933	-22.6	
<b>4aa</b>	1.211713	- 6033.29656 7	-6032.084854	-22.0	

<sup>a</sup>values given at B3LYP/6-31G(d) level at 40 °C and 1 atm. <sup>b</sup>values given at M062x/6-311++G(d,p) level in solvent chlorobenzene

**Table S3** Cartesian coordinates for the reaction of **1a** and **E1** at B3LYP/6-31G(d) level

<b>1a</b>				<b>E1</b>			
C	0.144493	2.590784	-1.059347	C	0.329062	1.175744	2.795521

C	0.200425	-2.567652	-1.051224	C	0.329064	-1.175733	2.795526
C	0.236644	0.749845	-2.642889	C	0.695952	2.58603	-1.013731
C	0.252737	-0.730352	-2.640508	C	0.695957	-2.586034	-1.013721
C	0.368676	2.592648	0.373519	C	0.800754	0.740239	-2.596139
C	0.424078	-2.559606	0.381644	C	0.800755	-0.740249	-2.596136
C	0.826645	1.455095	-1.61602	C	0.887386	2.583128	0.423914
C	0.858269	-1.419553	-1.611711	C	0.887391	-2.583126	0.423924
C	0.938285	0.764915	1.86338	C	1.375598	1.445935	-1.561907
C	0.953742	-0.714846	1.865341	C	1.375601	-1.44594	-1.561901
C	1.192994	1.460345	0.702772	C	1.39827	0.74022	1.923145
C	1.223597	-1.408598	0.707042	C	1.398271	-0.740211	1.923148
C	1.766429	0.833946	-0.576709	C	1.690877	1.442383	0.775083
C	1.784307	-0.774499	-0.574222	C	1.69088	-1.442378	0.775089
C	3.274619	1.208559	-0.87102	C	2.282296	0.810489	-0.496314
C	3.301068	-1.114739	-0.869736	C	2.282298	-0.810488	-0.496311
C	3.738559	2.532932	-0.296892	C	3.783643	1.208976	-0.784352
C	3.790531	-2.43611	-0.309958	C	3.783645	-1.208971	-0.78435
C	3.805434	3.663039	-1.119677	C	4.323174	2.525544	-0.28611
C	3.933428	-3.538865	-1.159464	C	4.323186	-2.525536	-0.286108
C	4.084396	-2.593895	1.052882	C	4.432457	2.833545	1.081266
C	4.089551	2.661243	1.055016	C	4.43249	-2.833529	1.081269
C	4.205736	4.89868	-0.606588	C	4.728974	3.476732	-1.232673
C	4.354775	-4.775129	-0.664321	C	4.728977	-3.476727	-1.232671
C	4.495815	3.892486	1.567835	C	4.939795	4.068031	1.48401
C	4.510731	-3.825394	1.548729	C	4.939837	-4.068011	1.484011
C	4.552903	5.016071	0.739153	C	5.223809	4.716566	-0.827009
C	4.645277	-4.921111	0.691756	C	5.223822	-4.716558	-0.827008
C	5.455482	0.078759	-0.822023	C	5.332544	5.012281	0.531864
C	6.445771	-0.099928	0.330124	C	5.332576	-5.012265	0.531865



C	7.896693	-0.042675	-0.12862	C	5.691704	0.000003	0.23882
C	8.957537	-0.219606	0.94522	C	-0.137451	-3.031253	1.262778
C	-0.092512	-1.160534	2.760106	C	-0.137457	3.031257	1.262766
C	-0.117662	1.190624	2.756544	C	-0.329417	0.000006	3.334148
C	-0.573192	-3.024639	1.245485	C	-0.423449	-2.310964	2.479422
C	-0.638513	3.03885	1.23581	C	-0.423453	2.310973	2.479413
C	-0.752552	0.008923	3.31072	C	-0.45806	-1.176463	-3.161164
C	-0.839107	-2.30673	2.467753	C	-0.458062	1.176449	-3.161169
C	-0.888916	2.319406	2.460478	C	-0.511695	-3.033587	-1.558567
C	-1.012124	-3.036225	-1.569726	C	-0.511701	3.033579	-1.558579
C	-1.015054	-1.181084	-3.172828	C	-1.10272	-2.311558	-2.658767
C	-1.04051	1.17138	-3.176622	C	-1.102725	2.311545	-2.658777
C	-1.077708	3.031446	-1.579562	C	-1.234079	-0.000008	-3.509298
C	-1.636442	-2.324235	-2.657852	C	-1.396874	-3.487941	0.697083
C	-1.686424	2.302532	-2.665345	C	-1.39688	3.487941	0.697069
C	-1.812627	-0.013864	-3.50376	C	-1.580389	-3.489039	-0.684381
C	-1.840074	-3.49429	0.707899	C	-1.580395	3.489033	-0.684395
C	-1.915299	3.478972	0.696549	C	-1.709186	0.000005	3.533559
C	-2.055187	-3.500568	-0.6695	C	-1.86114	-2.311654	2.677781
C	-2.12766	-0.00561	3.546756	C	-1.861144	2.31166	2.677772
C	-2.130547	3.476174	-0.680854	C	-2.464468	-3.040016	1.573795
C	-2.272128	-2.319515	2.696873	C	-2.464473	3.040017	1.573782
C	-2.321952	2.301764	2.689392	C	-2.492077	-1.177304	3.191629
C	-2.893183	-3.055695	1.607242	C	-2.492079	1.177312	3.191625
C	-2.904879	-1.191907	3.224741	C	-2.542708	-2.311754	-2.475662
C	-2.930317	1.162523	3.221006	C	-2.542712	2.311739	-2.475671
C	-2.958721	3.020675	1.597311	C	-2.617848	-0.000009	-3.340752
C	-3.071557	-2.336931	-2.440097	C	-2.838947	-3.040485	-1.253045
C	-3.121444	2.284958	-2.447596	C	-2.838952	3.040474	-1.253057

C	-3.193685	-0.028441	-3.308001	C	-3.285081	-1.177162	-2.80718
C	-3.331738	-3.065752	-1.208819	C	-3.285083	1.177144	-2.807184
C	-3.397338	3.012003	-1.218683	C	-3.673158	-2.603497	1.028996
C	-3.8354	-1.211803	-2.757482	C	-3.673162	2.603494	1.028986
C	-3.8608	1.142579	-2.761334	C	-3.75029	-0.727826	2.629767
C	-4.120248	-2.635103	1.090569	C	-3.750291	0.727829	2.629765
C	-4.17638	2.571947	1.082047	C	-3.864149	-2.6036	-0.412512
C	-4.180412	-0.757221	2.689712	C	-3.864153	2.603591	-0.412523
C	-4.19608	0.698556	2.687329	C	-4.329367	-1.425535	1.568102
C	-4.344009	-2.639976	-0.346329	C	-4.329369	1.425533	1.568096
C	-4.400213	2.567323	-0.354809	C	-4.354267	-0.727837	-1.937707
C	-4.77711	-1.46344	1.642864	C	-4.354268	0.727821	-1.93771
C	-4.807776	1.388213	1.638159	C	-4.637527	-1.425536	-0.762133
C	-4.888874	-0.772375	-1.863582	C	-4.63753	1.425524	-0.762138
C	-4.904538	0.683444	-1.865928	C	-4.92685	-0.697719	0.461728
C	-5.138125	-1.471089	-0.680292	C	-4.926852	0.697711	0.461725
C	-5.168863	1.380468	-0.684941	H	3.90128	1.185916	-1.873789
C	-5.407328	-0.744008	0.548934	H	3.90128	-1.185912	-1.873787
C	-5.422335	0.651759	0.546653	H	4.107603	2.120848	1.833119
H	3.355818	1.277925	-1.972675	H	4.107647	-2.120828	1.833122
H	3.383074	-1.175535	-1.972014	H	4.647684	-3.252553	-2.293574
H	3.544396	3.574924	-2.171844	H	4.647695	3.252553	-2.293575
H	3.714766	-3.429051	-2.219192	H	5.018807	4.295853	2.542734
H	3.978945	-1.74321	1.71823	H	5.018865	-4.295827	2.542735
H	4.042194	1.78792	1.69738	H	5.526005	5.445894	-1.572249
H	4.25264	5.764904	-1.26097	H	5.526011	-5.445888	-1.572248
H	4.4607	-5.619233	-1.340349	H	5.720681	5.975161	0.850155
H	4.73534	-3.931372	2.606908	H	5.72072	-5.975142	0.850156
H	4.766252	3.976233	2.617259	H	6.160858	-0.948116	0.482663

H	4.869648	5.975055	1.14022	H	6.16086	0.948122	0.482662
H	4.976699	-5.880493	1.079802	N	4.557052	0.000003	-0.342103
H	5.632004	-0.696688	-1.577583				
H	5.666755	1.031972	-1.315135				
H	6.278419	-1.053933	0.846084				
H	6.287449	0.678526	1.089016				
H	8.844115	0.539673	1.728997				
H	8.850793	-1.197779	1.430827	<b>H<sub>2</sub>O</b>			
H	9.951136	-0.140431	0.499461	H	0	0.76155	-0.478874
N	4.037932	0.055371	-0.385048	H	0	-0.76155	-0.478874
O	8.193854	0.133924	-1.296491	O	0	0	0.119718
<b>TS1a-H<sub>2</sub>O</b>				<b>TS1b-H<sub>2</sub>O</b>			
C	0.007003	0.735083	-2.616893	C	0.046178	-2.535808	-0.527889
C	0.01316	-0.745128	-2.609578	C	0.095847	0.762048	2.512754
C	0.090642	2.584766	0.396136	C	0.131206	-0.717657	2.503759
C	0.114785	-2.567195	0.420659	C	0.379439	0.798135	-2.039736
C	0.581606	1.439467	-1.580616	C	0.412684	-0.680979	-2.047293
C	0.594153	-1.434975	-1.567189	C	0.578825	1.476426	1.437536
C	0.619838	0.75805	1.901912	C	0.649302	-1.396011	1.421265
C	0.627061	-0.721664	1.909411	C	0.731737	1.493557	-0.905162
C	0.901219	1.448193	0.744145	C	0.797002	-1.373475	-0.92117
C	0.915261	-1.420319	0.758639	C	1.42733	0.869572	0.314415
C	1.497526	0.815836	-0.521487	C	1.467158	-0.735093	0.304909
C	1.503046	-0.792025	-0.513644	C	2.949106	1.265151	0.471852
C	3.015438	1.175885	-0.792158	C	3.011605	-1.060481	0.455299
C	3.022775	-1.142259	-0.773643	C	3.325447	2.598352	-0.145138
C	3.464219	2.522037	-0.258809	C	3.36167	3.748316	0.65184

C	3.489363	-2.454589	-0.172958	C	3.429266	-2.380582	-0.163092
C	3.538653	-3.609213	-0.962131	C	3.574576	-2.529521	-1.55052
C	3.644004	3.588101	-1.146641	C	3.613816	2.714079	-1.512156
C	3.674366	2.745105	1.109918	C	3.640036	-3.493628	0.658048
C	3.866312	-2.54389	1.176214	C	3.665771	4.992738	0.096456
C	3.947068	-4.83079	-0.421203	C	3.925704	-3.761919	-2.098059
C	4.021816	4.851176	-0.684575	C	3.92688	3.954244	-2.066533
C	4.055104	4.002707	1.574009	C	3.94941	5.098412	-1.26525
C	4.228377	5.061374	0.678026	C	3.986483	-4.731771	0.111216
C	4.281433	-3.762856	1.718244	C	4.130267	-4.868638	-1.269024
C	4.321763	-4.9114	0.919959	C	5.120907	0.214178	0.307136
C	5.185121	0.004735	-0.700433	C	6.090337	-0.565285	-0.589482
C	6.146085	0.473524	0.394347	C	7.544176	-0.2051	-0.33333
C	7.389148	1.015047	0.029044	C	8.539032	-1.207452	-0.362603
C	8.116233	1.969138	0.952484	C	-0.043528	-2.55091	0.919286
C	-0.081511	-2.57744	-1.016358	C	-0.073859	2.613617	-0.496949
C	-0.104674	2.580824	-1.040731	C	-0.165764	2.604603	0.950257
C	-0.439468	-1.158333	2.784705	C	-0.705171	-1.138641	-2.843694
C	-0.450473	1.192861	2.773137	C	-0.759747	1.21199	-2.830219
C	-0.902148	-3.023768	1.266027	C	-1.019829	-3.012512	-1.298052
C	-0.930046	3.039825	1.237494	C	-1.076475	-1.186251	3.148648
C	-1.103134	0.016852	3.31858	C	-1.131939	1.165594	3.163285
C	-1.187428	-2.300699	2.480875	C	-1.161887	3.049159	-1.261035
C	-1.208713	2.325538	2.459093	C	-1.197034	-3.037024	1.545479
C	-1.246507	-1.189939	-3.165425	C	-1.340096	3.028372	1.582785
C	-1.257048	1.162621	-3.176496	C	-1.40648	-2.295485	-2.488187
C	-1.286395	-3.040416	-1.557366	C	-1.427973	0.023233	-3.327297
C	-1.313937	3.027315	-1.585747	C	-1.514983	2.329717	-2.460155
C	-1.884834	-2.327852	-2.659482	C	-1.727821	-2.3362	2.689089

C	-1.905934	2.299116	-2.681208	C	-1.83673	2.289293	2.717598
C	-2.030122	-0.01881	-3.51521	C	-1.855289	-0.030488	3.555495
C	-2.161298	-3.486926	0.704879	C	-2.225478	-3.500316	-0.647828
C	-2.193168	3.486403	0.672353	C	-2.312556	-3.513018	0.743493
C	-2.349644	-3.495936	-0.676421	C	-2.389243	3.470663	-0.604591
C	-2.381376	3.480936	-0.708989	C	-2.476792	3.461878	0.786745
C	-2.482646	0.011525	3.527863	C	-2.818628	-0.009049	-3.435631
C	-2.62481	-2.303988	2.681855	C	-2.854166	-2.326725	-2.584386
C	-2.645913	2.317433	2.660161	C	-2.962723	2.293369	-2.555787
C	-3.228998	-3.039343	1.582261	C	-3.176655	-2.367378	2.604363
C	-3.25678	3.037082	1.553846	C	-3.24821	-0.062749	3.488203
C	-3.260736	-1.170946	3.193966	C	-3.285395	2.253563	2.633047
C	-3.271587	1.183595	3.183216	C	-3.36256	-3.07353	-1.444736
C	-3.324015	-2.331362	-2.469914	C	-3.505328	3.00093	-1.406945
C	-3.344997	2.290728	-2.491339	C	-3.539651	-3.096603	1.399604
C	-3.414809	-0.024528	-3.346482	C	-3.547369	-1.206322	-3.047727
C	-3.612697	-3.055023	-1.241923	C	-3.602792	1.147568	-3.033209
C	-3.640338	3.023016	-1.270058	C	-3.682626	2.979937	1.437344
C	-4.074412	-1.20242	-2.805243	C	-3.922608	-1.2532	2.994884
C	-4.08531	1.152079	-2.816338	C	-3.97793	1.100765	3.009504
C	-4.443102	-2.612745	1.040421	C	-4.542334	-2.670771	-0.815851
C	-4.46694	2.594432	1.016227	C	-4.632563	-2.682032	0.635485
C	-4.522821	-0.729948	2.632785	C	-4.664637	2.535209	-0.783417
C	-4.529453	0.725862	2.626071	C	-4.755044	2.524105	0.667903
C	-4.638889	-2.62047	-0.400519	C	-4.77359	-0.789842	-2.395811
C	-4.662668	2.587022	-0.424727	C	-4.807852	0.66562	-2.386792
C	-5.103387	-1.435506	1.576501	C	-5.059386	-0.825486	2.20325
C	-5.116373	1.41624	1.563275	C	-5.09355	0.630021	2.212246
C	-5.14241	-0.753959	-1.933312	C	-5.26223	-1.50645	-1.301092

C	-5.149039	0.701914	-1.940103	C	-5.329353	1.344589	-1.283333
C	-5.419097	-1.447693	-0.753199	C	-5.407605	-1.524497	1.045375
C	-5.432064	1.403952	-0.766457	C	-5.474667	1.326396	1.063163
C	-5.707829	-0.715454	0.468512	C	-5.798259	-0.798056	-0.151238
C	-5.714021	0.680377	0.462007	C	-5.830993	0.597388	-0.142541
H	3.117449	1.213872	-1.893793	H	3.12764	1.338148	1.562042
H	3.1286	-1.223328	-1.872651	H	3.150301	3.669196	1.7159
H	3.26014	-3.55103	-2.011607	H	3.198084	-1.131484	1.544471
H	3.489915	3.428568	-2.211394	H	3.427032	-1.667944	-2.193198
H	3.542962	1.924438	1.807184	H	3.53498	-3.390768	1.735705
H	3.836896	-1.649308	1.789907	H	3.601368	1.822409	-2.130592
H	3.980054	-5.715276	-1.051371	H	3.688377	5.875514	0.729863
H	4.158527	5.665419	-1.391089	H	4.040292	-3.85973	-3.174411
H	4.216558	4.15792	2.637588	H	4.147938	-5.58429	0.765445
H	4.525045	6.041583	1.041607	H	4.154598	4.027805	-3.126677
H	4.565176	-3.817573	2.766237	H	4.192779	6.064467	-1.69934
H	4.643138	-5.859176	1.34298	H	4.40293	-5.829208	-1.69782
H	5.315556	0.620299	-1.606454	H	5.251828	-0.097301	1.36032
H	5.411448	-1.018379	-1.019405	H	5.411195	1.264206	0.251812
H	5.670725	0.907667	1.268227	H	5.875525	-0.313466	-1.637922
H	6.376306	-2.560126	0.913465	H	5.967729	-1.645516	-0.498236
H	6.732073	-0.905108	0.844997	H	8.24062	-2.179014	-0.751091
H	7.515975	-1.967007	-0.314426	H	8.878531	1.188986	0.564186
H	7.615229	2.082086	1.917458	H	8.900468	-1.283271	1.056096
H	7.859586	-0.556435	-1.416755	H	9.526709	-0.879264	-0.693741
H	8.164317	2.953308	0.470137	H	9.603451	1.900062	1.95993
H	8.734407	-1.970927	-1.666432	H	9.670906	0.146819	1.820847
H	9.148213	1.636048	1.106891	H	10.183904	-1.54529	2.197729
N	3.761027	0.021826	-0.278072	N	3.696432	0.124187	-0.076035

O	7.147312	-1.968602	0.820056	O	7.783102	1.020145	-0.037566
O	7.824073	-1.683594	-1.489115	O	9.366729	-1.023434	2.128937
O	8.007744	0.70743	-1.057226	O	9.793279	1.211352	1.302436
<b>TS1a-TsOH</b>				<b>TS1b-TsOH</b>			
C	0.261663	0.863175	0.089952	C	0.020921	1.052506	0.13831
C	0.328914	-0.72505	-0.130719	C	0.396807	-1.478278	0.795907
C	1.7891	1.300436	0.10464	C	0.648855	-0.941448	-1.475869
C	1.87808	-1.019495	-0.203672	C	0.716541	1.295614	1.482437
C	1.966404	3.012676	-1.776374	C	0.78101	-1.114404	2.068597
C	2.0139	2.711909	-0.40619	C	0.945478	0.313637	2.42204
C	2.071943	4.330362	-2.217898	C	0.967312	1.827135	-0.790684
C	2.187694	3.759281	0.505343	C	1.058106	-2.577585	0.148434
C	2.229773	5.371812	-1.297547	C	1.216268	-2.244935	-1.254212
C	2.26479	-2.204646	-1.067576	C	1.279575	-0.078392	-2.343678
C	2.294176	5.08205	0.065609	C	1.443276	1.349377	-1.990887
C	2.365133	-2.08812	-2.46123	C	1.630624	2.399708	1.380771
C	2.507458	-3.448437	-0.47413	C	1.787607	2.726436	-0.023511
C	2.693231	-3.19562	-3.241387	C	1.81499	-1.855937	2.75763
C	2.828645	-4.560257	-1.254978	C	2.040959	-3.324707	0.807573
C	2.921229	-4.43638	-2.641056	C	2.075849	0.413555	3.319692
C	3.946111	0.200351	-0.36381	C	2.351544	-2.67556	-1.94908
C	4.785212	1.152365	-1.219498	C	2.429953	-2.954029	2.146192
C	5.30349	2.365573	-0.745924	C	2.471542	-0.491769	-3.052384
C	5.58342	3.539225	-1.629406	C	2.612835	-0.919127	3.527975
C	8.948788	-0.733446	0.781545	C	2.713964	2.529132	2.257216
C	9.613525	0.446462	1.120688	C	2.73215	1.776701	-2.491051
C	9.645043	-1.932343	0.635329	C	2.943059	1.509507	3.251524

C	-0.326382	-1.548664	0.984143	C	2.996875	-1.775689	-2.87318
C	-0.447021	1.293698	1.381158	C	3.023998	3.17452	-0.500644
C	-0.476403	-1.23293	-1.337373	C	3.229579	-3.754639	0.089073
C	-0.605619	1.604131	-0.940312	C	3.366477	0.647065	-3.14527
C	-0.709808	-1.032611	2.202839	C	3.381309	-3.436398	-1.259684
C	-0.774568	0.431818	2.405959	C	3.509912	2.687335	-1.768221
C	-1.019542	-0.421273	-2.307374	C	3.863435	-3.146847	2.268738
C	-1.0494	-2.658955	0.429373	C	3.988398	-1.109634	3.658598
C	-1.086757	1.042149	-2.101345	C	4.0034	2.976245	1.755928
C	-1.145691	-2.462355	-1.004089	C	4.154701	3.29125	0.40636
C	-1.275396	2.443354	1.139826	C	4.359475	-3.643088	0.994918
C	-1.374669	2.633853	-0.294198	C	4.376028	1.312279	3.37291
C	-1.812597	-1.623799	2.92908	C	4.431392	-1.96581	-2.762148
C	-1.916342	0.704067	3.252308	C	4.628198	-2.242688	3.008915
C	-2.100146	-3.263276	1.128832	C	4.670532	-2.995108	-1.763005
C	-2.221887	-0.817654	-3.008226	C	4.746847	0.465737	-3.054232
C	-2.292771	-2.879239	-1.687984	C	4.889286	0.02882	3.571436
C	-2.326604	1.508626	-2.683116	C	4.943833	2.492571	-1.658026
C	-2.367474	2.739872	1.963533	C	5.033522	2.22066	2.446909
C	-2.492817	-2.731234	2.410788	C	5.289914	-0.867761	-2.849723
C	-2.556642	-0.558191	3.575959	C	5.344393	2.867179	-0.311173
C	-2.561154	3.119878	-0.853417	C	5.551097	1.403712	-2.287378
C	-2.696988	1.846971	3.047405	C	5.598603	-3.215106	0.513965
C	-2.846326	-2.035196	-2.718208	C	5.75728	-2.884754	-0.893314
C	-3.026946	0.367185	-3.242302	C	5.916325	-1.801612	2.510862
C	-3.051005	2.542479	-2.080885	C	6.077658	-0.397095	2.858544
C	-3.29927	-3.678327	0.419426	C	6.176045	1.808633	1.757973
C	-3.39327	-3.489024	-0.958584	C	6.334834	2.138887	0.350767
C	-3.607211	3.225117	1.378845	C	6.392667	-2.276807	1.287018



C	-3.701666	3.410859	0.000427	C	6.419874	-0.755084	-1.948294
C	-3.939198	-2.806804	2.506027	C	6.581604	0.649447	-1.600731
C	-3.945473	-0.634833	3.680783	C	6.64975	-1.742884	-0.988103
C	-4.143384	1.766962	3.141808	C	6.70879	0.474296	1.968208
C	-4.293374	-2.108624	-2.633839	C	6.96615	1.008232	-0.306873
C	-4.418913	0.296476	-3.177796	C	7.043559	-1.367206	0.359123
C	-4.439541	-3.39365	1.272973	C	7.198429	-0.020659	0.692547
C	-4.497744	2.46451	-1.998022	C	-0.158442	-0.499971	-0.245964
C	-4.633185	-3.009957	-1.544335	C	-1.464778	1.593585	0.159152
C	-4.652118	-1.779252	3.127383	C	-1.591775	3.515359	-1.507369
C	-4.707885	2.62069	2.10872	C	-1.631469	3.061399	-0.180617
C	-4.756082	0.550694	3.450912	C	-1.725555	-0.653911	-0.393948
C	-4.901919	3.002823	-0.708919	C	-1.731515	4.872131	-1.79634
C	-5.065123	-0.966389	-2.858213	C	-1.814646	3.995304	0.845386
C	-5.169026	1.363484	-2.534298	C	-1.907727	5.796971	-0.763891
C	-5.630928	-2.929075	0.712265	C	-1.948043	5.355482	0.558382
C	-5.729888	-2.7338	-0.725402	C	-2.122407	-1.572826	-2.738931
C	-5.861044	2.224057	1.428239	C	-2.191901	-1.736946	-1.346944
C	-5.890977	-1.299798	2.546656	C	-2.54376	-2.589555	-3.594992
C	-5.955249	0.140872	2.746734	C	-2.691392	-2.940466	-0.836809
C	-5.96008	2.419221	-0.009443	C	-3.036758	-3.78915	-3.073998
C	-6.205143	-0.681088	-2.008972	C	-3.10891	-3.962682	-1.692296
C	-6.269583	0.759576	-1.808872	C	-3.656354	0.84807	-0.657786
C	-6.37116	-1.861931	1.36173	C	-4.307515	1.106275	-2.039256
C	-6.49705	0.959957	1.753737	C	-5.797175	1.218607	-1.913727
C	-6.531869	-1.546388	-0.962505	C	-6.688203	0.226998	-2.341024
C	-6.657711	1.275569	-0.5704	C	-9.846422	-0.373195	1.030888
C	-6.929191	-1.007438	0.32711	C	-10.088228	-1.012621	2.246643
C	-6.990942	0.373771	0.519035	C	-10.827828	-0.325842	0.039627

C	10.992498	0.417374	1.30902	C	-11.326373	-1.614686	2.46344
C	11.025939	-1.942408	0.827091	C	-12.059992	-0.931051	0.274163
C	11.720196	-0.773803	1.166454	C	-12.329874	-1.583855	1.485853
C	13.21141	-0.799149	1.404551	C	-13.68077	-2.208804	1.74194
H	1.843286	2.204504	-2.489693	H	-1.451019	2.796845	-2.308481
H	2.025399	4.54726	-3.281988	H	-1.701145	5.208873	-2.829268
H	2.100051	1.275149	1.166062	H	-1.737731	-0.642548	-3.14429
H	2.188454	-1.245651	0.833182	H	-1.820735	1.450179	1.196492
H	2.195162	-1.121335	-2.924166	H	-1.857196	3.655302	1.877559
H	2.234142	3.540512	1.569431	H	-2.017499	6.853961	-0.990626
H	2.303174	6.399746	-1.642555	H	-2.092035	6.065688	1.367959
H	2.423943	5.88177	0.789716	H	-2.095013	-0.922377	0.613589
H	2.452819	-3.546559	0.6074	H	-2.483792	-2.44714	-4.670865
H	2.772993	-3.090039	-4.320177	H	-2.758681	-3.078227	0.2398
H	3.018426	-5.517462	-0.777316	H	-3.364276	-4.580911	-3.742299
H	3.17865	-5.298501	-3.250428	H	-3.496477	-4.888666	-1.276594
H	4.141622	0.367007	0.706898	H	-3.902243	1.688624	-0.003028
H	4.270454	-0.821847	-0.573391	H	-3.920693	2.053269	-2.432716
H	4.475614	1.179079	-2.262338	H	-4.049228	0.30681	-2.73492
H	4.96902	4.38145	-1.289811	H	-4.106984	-0.046713	-0.209398
H	5.339675	3.32914	-2.671392	H	-6.28619	-0.53437	-3.00395
H	5.877155	1.667393	0.964627	H	-7.002112	-0.340463	-1.139488
H	5.993266	0.499386	-1.169267	H	-7.138955	2.146901	-0.901697
H	6.633615	3.835376	-1.537781	H	-7.708799	0.543638	-2.556054
H	9.055131	1.368188	1.24615	H	-9.317897	-1.02545	3.010201
H	9.106181	-2.839177	0.382791	H	-10.632261	0.192146	-0.893106
H	11.513927	1.333929	1.574773	H	-11.517136	-2.113836	3.410416
H	11.572491	-2.875464	0.713429	H	-12.827596	-0.892729	-0.495202
H	13.438	-0.935586	2.470371	H	-13.611848	-3.032787	2.459497

H	13.683759	0.137739	1.090505	H	-14.12477	-2.596895	0.819156
H	13.690195	-1.620481	0.861817	H	-14.383022	-1.473135	2.156179
N	2.494053	0.24772	-0.635899	N	-2.190744	0.693008	-0.744368
O	5.711921	2.543686	0.488244	O	-6.18527	2.262955	-1.223728
O	6.603985	0.289078	1.456482	O	-7.434724	-0.7367	-0.011856
O	6.675592	-2.080057	0.61959	O	-7.638771	0.667228	2.04199
O	7.06642	-0.151858	-0.945133	O	-8.473798	1.510473	-0.188719
S	7.184501	-0.711595	0.499033	S	-8.239529	0.355798	0.744144
<b>G1</b>				<b>I1</b>			
C	0.40052	-3.032634	1.189708	C	0.408571	-3.011658	1.241344
C	0.400908	3.032674	1.189773	C	0.450983	3.051722	1.172846
C	0.406733	-0.000002	3.264882	C	0.47211	0.043417	3.282123
C	0.575222	-2.313022	2.42744	C	0.609932	-2.279777	2.467699
C	0.575518	2.313014	2.42749	C	0.64224	2.345413	2.415771
C	1.028637	-3.034772	-1.589293	C	0.987744	-3.050206	-1.547636
C	1.029026	3.034793	-1.589226	C	1.030811	3.017657	-1.616449
C	1.119316	-1.176272	-3.186742	C	1.063775	-1.211248	-3.167841
C	1.119467	1.176315	-3.186717	C	1.080566	1.141148	-3.194569
C	1.70593	-3.487571	0.738472	C	1.662986	-2.346148	-2.6102
C	1.706376	3.487455	0.738547	C	1.695704	2.279897	-2.662642
C	1.716941	-2.313385	-2.631742	C	1.702466	-3.481637	0.773017
C	1.717237	2.31334	-2.631691	C	1.751555	3.491828	0.693682
C	1.762801	-0.000093	3.592687	C	1.833657	0.037079	3.586244
C	1.924631	-0.000027	-3.461646	C	1.872469	-0.043983	-3.470171
C	1.989617	-2.310784	2.752691	C	1.986278	-3.501048	-0.591759
C	1.989913	2.310588	2.752741	C	2.029633	-2.284615	2.768721
C	2.013677	-3.489433	-0.621316	C	2.035672	3.476322	-0.671123

C	2.014125	3.489307	-0.62124	C	2.062129	2.336336	2.716179
C	2.572857	-1.177294	3.32299	C	2.630584	-1.148951	3.315769
C	2.573007	1.177011	3.323015	C	2.647266	1.205143	3.289102
C	2.690969	-3.038758	1.707187	C	2.707384	-3.029389	1.719483
C	2.691358	3.038494	1.707253	C	2.750181	3.047018	1.650202
C	3.134241	-2.311253	-2.318039	C	3.085549	-2.350734	-2.321066
C	3.134538	2.31102	-2.317989	C	3.118169	2.271083	-2.373552
C	3.289459	-0.000117	-3.173677	C	3.241992	-0.050556	-3.205529
C	3.318688	-3.039358	-1.072758	C	3.286438	-3.065946	-1.070908
C	3.319078	3.039075	-1.072692	C	3.329427	3.011844	-1.140051
C	3.877077	-0.728177	2.876254	C	3.85986	-1.225499	-2.611317
C	3.87717	0.727737	2.876269	C	3.876514	1.128783	-2.638203
C	3.905415	-1.177427	-2.582183	C	3.929893	-0.714391	2.841296
C	3.905566	1.177101	-2.582157	C	3.940185	0.741385	2.824763
C	3.945562	-2.604151	1.274997	C	3.957216	-2.608779	1.260584
C	3.945896	2.603737	1.275054	C	3.993923	2.598484	1.201264
C	4.265713	-2.604115	-0.143499	C	4.252507	-2.627047	-0.163187
C	4.266047	2.60369	-0.143443	C	4.289347	2.580185	-0.22247
C	4.550594	-1.426154	1.871306	C	4.580861	-1.428571	1.832867
C	4.550776	1.425649	1.871337	C	4.601003	1.423001	1.800391
C	4.891263	-0.728148	-1.618794	C	4.86555	-0.772503	-1.670447
C	4.891356	0.727675	-1.618778	C	4.875801	0.683199	-1.68702
C	5.067699	-1.426118	-0.422053	C	5.057847	-1.458164	-0.469028
C	5.067882	1.425596	-0.422022	C	5.077886	1.393254	-0.501498
C	5.24529	-0.698193	0.823171	C	5.262257	-0.717531	0.764555
C	5.245379	0.697621	0.823186	C	5.27203	0.678146	0.748652
C	-0.186724	0.740673	-2.741421	C	-0.138892	1.216872	2.685208
C	-0.186819	-0.740472	-2.741437	C	-0.154919	-1.134353	2.711186
C	-0.202019	1.175865	2.670434	C	-0.214003	2.577119	-1.153417

C	-0.20217	-1.175779	2.670409	C	-0.220389	0.719689	-2.72138
C	-0.220832	2.580851	-1.153477	C	-0.231324	-0.76103	-2.704833
C	-0.221163	-2.580681	-1.153534	C	-0.25121	-2.582159	-1.095755
C	-0.540913	2.577964	0.261026	C	-0.510131	2.593035	0.266078
C	-0.541241	-2.577782	0.260969	C	-0.545644	-2.560089	0.323927
C	-0.852414	1.439816	-1.757233	C	-0.862855	1.433476	-1.732645
C	-0.852599	-1.43955	-1.757264	C	-0.88544	-1.443841	-1.701633
C	-1.190104	0.740332	1.707264	C	-1.147178	0.777852	1.744674
C	-1.190199	-0.740098	1.707248	C	-1.156323	-0.702072	1.760305
C	-1.373496	1.436764	0.53374	C	-1.346556	1.461532	0.5665
C	-1.373677	-1.43648	0.533708	C	-1.365343	-1.409898	0.597882
C	-1.849338	0.805985	-0.782165	C	-1.848568	0.817447	-0.734077
C	-1.849437	-0.805613	-0.782182	C	-1.861878	-0.790541	-0.716627
C	-3.342624	1.149243	-1.16236	C	-3.340808	1.173741	-1.100308
C	-3.342778	-1.148659	-1.162396	C	-3.36288	-1.130601	-1.077937
C	-3.83008	2.531927	-0.778188	C	-3.786085	3.574106	-1.660004
C	-3.83041	-2.531321	-0.778365	C	-3.798971	2.560103	-0.691934
C	-3.86064	3.519896	-1.772802	C	-3.829234	-2.5133	-0.66399
C	-3.86134	-3.519106	-1.773155	C	-3.958521	-3.493162	-1.657109
C	-4.218194	2.879661	0.52424	C	-4.084232	-2.874399	0.668809
C	-4.218316	-2.87923	0.524074	C	-4.148698	4.882029	-1.336285
C	-4.257444	4.8251	-1.480151	C	-4.198186	2.882682	0.613792
C	-4.258313	-4.824292	-1.480667	C	-4.330063	-4.800373	-1.336924
C	-4.623511	4.182678	0.814769	C	-4.464541	-4.177323	0.988799
C	-4.623799	-4.182232	0.814447	C	-4.544241	5.192282	-0.03515
C	-4.641596	5.160018	-0.181848	C	-4.572724	4.187867	0.934062
C	-4.64226	-5.159383	-0.182346	C	-4.584575	-5.145955	-0.010512
C	-5.545013	0.000434	-1.004951	C	-5.541239	0.07909	-1.013557
C	-6.226521	-0.000399	1.471135	C	-6.524427	-0.021454	1.352879

C	-6.50733	-0.000315	0.15693	C	-6.534333	-0.595934	-0.047343
C	-7.262913	-0.001082	2.555401	C	-7.619097	0.383499	2.005079
H	-3.383589	1.098174	-2.265472	H	-3.391418	1.13384	-2.203597
H	-3.383724	-1.097504	-2.265505	H	-3.41385	-1.100751	-2.181432
H	-3.567462	3.264103	-2.788553	H	-3.485634	3.337152	-2.678178
H	-3.568318	-3.263174	-2.788917	H	-3.763079	-3.230955	-2.694378
H	-4.218685	-2.13803	1.314889	H	-4.018856	-2.135497	1.45919
H	-4.218863	2.138315	1.314919	H	-4.128938	5.65268	-2.102097
H	-4.27149	5.574269	-2.267131	H	-4.242915	2.117321	1.380036
H	-4.272646	-5.573318	-2.267779	H	-4.42373	-5.542692	-2.124861
H	-4.355171	0.000244	1.198844	H	-4.618616	-0.011686	1.247853
H	-4.927252	4.432598	1.827756	H	-4.668468	-4.434147	2.024601
H	-4.927374	-4.432285	1.82745	H	-4.834653	6.207632	0.220858
H	-4.956963	6.173468	0.051352	H	-4.878381	-6.160547	0.244361
H	-4.957753	-6.172823	0.050726	H	-4.889911	4.416996	1.947627
H	-5.738545	-0.876077	-1.639679	H	-5.633873	-0.368074	-2.01674
H	-5.73863	0.877707	-1.638586	H	-5.814354	1.133811	-1.101799
H	-7.142798	-0.882862	3.197065	H	-6.325976	-1.670132	0.001658
H	-7.143176	0.880231	3.197771	H	-7.537415	-0.484411	-0.472538
H	-7.556195	-0.000717	-0.127684	H	-7.554975	0.762679	3.019456
H	-8.274515	-0.001139	2.141891	H	-8.596844	0.3196	1.542082
N	-4.100332	0.00033	-0.623071	N	-4.121389	0.033536	-0.56586
O	-4.956753	0.000039	1.987063	O	-5.295129	0.015377	1.96538
<b>TS2a</b>				<b>TS2b</b>			
C	0.294966	1.729703	0.113989	C	0.720401	0.798803	0.910021
C	1.348414	2.23772	1.124239	C	1.845608	-3.158907	4.145892
C	1.759247	-1.507873	4.364071	C	1.90908	-2.885513	2.777131

C	2.016931	-1.177438	3.031118	C	2.032578	1.612326	2.367324
C	2.123041	-0.63033	5.385014	C	2.508317	-2.327806	5.048151
C	2.652746	0.025981	2.70355	C	2.534586	4.269533	-1.197424
C	2.746023	0.579662	5.067055	C	2.63176	-1.787677	2.311514
C	2.955826	0.345686	1.253624	C	2.633337	5.581165	-0.723594
C	3.006641	3.635086	-2.278515	C	3.065553	3.212453	-0.458104
C	3.012557	0.904354	3.737849	C	3.226863	-1.225332	4.581947
C	3.027493	4.947801	-2.756456	C	3.267017	5.830113	0.493204
C	3.253957	1.920686	-0.448183	C	3.29993	-0.940371	3.211281
C	3.271274	3.356648	-0.930762	C	3.703083	3.450829	0.770962
C	3.305424	6.001974	-1.884645	C	3.793996	4.770602	1.234505
C	3.562257	4.421813	-0.067125	C	4.098886	0.266306	2.771612
C	3.57316	5.734153	-0.539756	C	4.292311	2.346445	1.620577
C	4.45384	0.112316	0.795011	C	5.062217	-1.097238	-0.473269
C	4.659989	1.199805	-0.374497	C	5.181822	0.193625	-1.186901
C	4.681194	-1.339962	0.357947	C	5.257776	-1.163632	0.888492
C	4.796671	-1.739761	-0.956269	C	5.340444	0.061321	1.814218
C	4.98553	-0.739379	-2.031955	C	5.471942	1.473291	1.033322
C	5.048719	0.605028	-1.733409	C	5.489851	1.346619	-0.499137
C	5.386325	-2.062995	1.380307	C	5.593417	-2.125974	-1.341916
C	5.479673	0.211138	1.93402	C	5.78338	-0.075013	-2.475769
C	5.590104	-2.901175	-1.297533	C	6.036409	-1.50058	-2.574228
C	5.843351	2.153903	-0.151941	C	6.038114	-2.243901	1.431939
C	5.880328	-1.105811	2.351823	C	6.313031	-3.200367	-0.809953
C	5.889416	-1.312029	-3.006414	C	6.454875	2.257631	-1.056237
C	6.043378	1.424076	-2.369505	C	6.541365	-3.259574	0.613099
C	6.137822	-3.202893	1.074169	C	6.576019	-0.319048	2.644756
C	6.242875	-3.632457	-0.299074	C	6.686551	0.831911	-3.038825
C	6.262575	-2.641423	-2.557782	C	6.809301	2.197009	1.253896

C	6.351619	1.262543	2.105261	C	6.84787	-1.723234	2.516364
C	6.535506	2.377698	-1.393375	C	7.031083	2.027856	-2.309596
C	6.539217	2.263201	1.030952	C	7.178191	-1.9664	-3.225609
C	6.831129	-0.508371	-3.65848	C	7.265304	2.783917	0.025116
C	6.909462	0.894681	-3.332571	C	7.507251	-3.681451	-1.479785
C	7.107607	-1.326571	2.985021	C	7.606379	0.549036	2.932348
C	7.421223	-3.422801	1.721221	C	7.726176	1.840375	2.218253
C	7.556098	-3.116341	-2.773067	C	7.879325	-3.782657	0.838448
C	7.593214	-4.11868	-0.516681	C	7.880821	0.351163	-3.70895
C	7.637541	1.052481	2.734853	C	7.933151	-3.074902	-2.663018
C	7.878254	2.76851	-1.418822	C	8.123502	-1.020889	-3.798119
C	7.895679	-2.503603	2.655602	C	8.130537	-2.234082	2.740646
C	7.936327	2.64133	1.027342	C	8.442975	2.301767	-2.524845
C	8.010064	-0.218947	3.18279	C	8.477886	-4.041995	-0.459137
C	8.181012	-0.996448	-3.87482	C	8.620835	3.058081	-0.184675
C	8.238021	-3.86443	-1.728717	C	8.657601	-3.280475	1.87985
C	8.308497	1.290073	-3.34771	C	8.945351	0.04333	3.146069
C	8.323299	-3.989218	0.734096	C	8.969158	1.26108	-3.390459
C	8.537305	-2.274067	-3.438914	C	9.135614	2.095606	2.011686
C	8.598	2.904674	-0.176409	C	9.205886	-1.328491	3.063653
C	8.613818	1.89982	2.075145	C	9.221473	2.80573	-1.484445
C	8.782109	2.206214	-2.409966	C	9.341915	-2.808743	-2.877367
C	9.096331	0.116932	-3.682487	C	9.459586	-1.538841	-3.579255
C	9.294308	-2.112291	2.647355	C	9.579614	2.705467	0.833742
C	9.364288	-0.697023	2.973523	C	9.833797	-3.780755	-0.663639
C	9.634692	-3.476279	-1.742157	C	9.887585	0.992193	2.581124
C	9.666983	-3.610182	0.720957	C	-0.45975	1.456077	1.20054
C	9.819749	-2.493069	-2.799623	C	-0.924921	2.696914	0.511482
C	9.919449	1.447766	1.883582	C	-1.083991	-2.197752	-2.421852



C	9.95198	2.424704	-0.383782	C	-1.154023	-1.763395	-3.745708
C	-0.160447	2.591023	-0.87628	C	-1.720397	-1.470679	-1.413699
C	-0.598118	2.17538	-2.249755	C	-1.771535	2.501907	-0.80592
C	-0.799986	-3.487191	0.745557	C	-1.867388	-0.602767	-4.055877
C	-0.911817	-3.724407	2.116049	C	-2.445447	-0.311527	-1.715261
C	-1.284451	1.388589	1.458143	C	-2.512794	0.115528	-3.049899
C	-1.377802	-2.345357	0.186889	C	-3.15653	0.434357	-0.604691
C	-1.599963	-2.815402	2.92437	C	-4.007635	2.435858	0.266054
C	-2.081302	-1.435794	0.986727	C	-4.235094	3.929671	0.153006
C	-2.184408	-1.680097	2.365107	C	-4.323867	4.709634	1.312244
C	-2.747272	-0.246892	0.331822	C	-4.383363	4.553112	-1.095013
C	-3.432369	2.046991	0.456857	C	-4.562396	6.083352	1.233087
C	-3.497676	4.554421	0.58084	C	-4.61203	5.926094	-1.175808
C	-3.511709	3.328406	1.256382	C	-4.704352	6.69479	-0.012526
C	-3.608344	5.756331	1.281747	C	-4.709619	0.148923	-0.471477
C	-3.630837	3.325178	2.654852	C	-4.968851	-1.086759	0.398785
C	-3.718691	5.743853	2.672173	C	-5.292962	1.522289	0.132433
C	-3.726716	4.526062	3.356682	C	-5.319863	-2.211104	-0.424077
C	-4.319836	-0.299269	0.17512	C	-5.380688	-0.300289	-1.778318
C	-4.692962	-1.006152	-1.13627	C	-5.42083	-1.03179	1.699843
C	-4.780634	1.244443	0.255142	C	-5.57657	-1.725628	-1.766606
C	-5.023544	-1.221859	1.184946	C	-5.955785	0.232441	2.256168
C	-5.138298	-2.345181	-0.86884	C	-6.008878	1.370914	1.480312
C	-5.144725	-0.350394	-2.260897	C	-6.061453	-3.280692	0.089603
C	-5.344527	-2.477683	0.560674	C	-6.211158	-2.115681	2.242913
C	-5.515423	1.753845	-0.993703	C	-6.229364	0.485484	-2.525079
C	-5.567329	1.067094	-2.187621	C	-6.420171	2.152446	-0.699141
C	-5.797364	-0.776418	2.232697	C	-6.519187	-3.231472	1.456854
C	-5.845197	1.532735	1.327469	C	-6.565828	-2.331352	-2.547948

C	-5.975538	-3.019115	-1.764202	C	-6.764609	1.748427	-1.96914
C	-6.029958	-1.022028	-3.1881	C	-7.061118	-0.107603	3.126746
C	-6.219852	0.640142	2.306064	C	-7.100278	-3.899001	-0.718159
C	-6.381761	-3.282818	1.041462	C	-7.185339	2.195397	1.514722
C	-6.432934	-2.340848	-2.952488	C	-7.220231	-1.550649	3.120495
C	-6.61275	2.599283	-0.613277	C	-7.276552	-0.117868	-3.3212
C	-6.70165	1.230079	-3.071804	C	-7.347297	-3.43306	-2.00854
C	-6.817558	2.461443	0.816049	C	-7.4386	-1.506732	-3.346988
C	-6.889753	-1.583361	2.732295	C	-7.440148	2.675714	0.169957
C	-6.988112	-0.052757	-3.688253	C	-7.847317	-3.815097	1.50842
C	-7.061729	-3.845136	-1.262748	C	-8.12639	1.889113	-2.438297
C	-7.174418	-2.825225	2.1563	C	-8.190262	0.716005	3.193471
C	-7.260517	-3.973314	0.110759	C	-8.207648	-4.228583	0.161704
C	-7.561044	0.66723	2.848778	C	-8.253516	1.897357	2.367785
C	-7.707293	2.786909	-1.4641	C	-8.443688	0.743475	-3.270848
C	-7.753079	2.084769	-2.723567	C	-8.493947	-2.1157	3.179222
C	-7.807779	-2.737697	-3.196283	C	-8.712959	-3.279492	-2.478548
C	-7.975196	-0.698406	3.112925	C	-8.756626	2.843269	-0.271225
C	-8.112302	2.51873	1.341243	C	-8.768811	-2.085876	-3.307089
C	-8.197583	-3.669122	-2.15013	C	-8.81632	-3.26723	2.351283
C	-8.307316	-0.433653	-3.930939	C	-9.109646	2.440367	-1.610402
C	-8.494243	1.599652	2.385237	C	-9.5176	0.130562	3.244244
C	-8.550822	-3.223608	1.925987	C	-9.521183	-4.076177	-0.286229
C	-8.604805	-3.934882	0.659115	C	-9.621674	2.057068	1.902402
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C	-9.127613	1.687041	-2.967534	C	-9.778904	-3.592586	-1.633136
C	-9.251355	2.701085	0.455645	C	-9.867	2.518793	0.610218
C	-9.299105	-1.082409	2.902116	C	-9.889406	-1.254583	-3.255316

C	-9.399515	0.451215	-3.557098	C	10.069434	-3.012535	1.670653
C	-9.490097	-3.625853	-1.624583	C	10.254517	0.761378	-3.174148
C	-9.592708	-2.36829	2.289369	C	10.274353	-3.152821	-1.896757
C	-9.69779	-3.761738	-0.191765	C	10.408401	-1.803692	2.40389
C	-9.870624	1.200774	2.154837	C	10.504761	-0.665777	-3.27135
C	-9.933401	2.150212	-1.849494	C	10.56084	2.291015	-1.260895
C	10.066872	1.9923	-1.767292	C	10.645513	-3.255561	0.422536
C	10.1624	-2.653204	1.697279	C	10.782048	2.229042	0.174733
C	10.300333	0.118932	2.335245	C	11.047903	0.538664	1.95505
C	10.329075	-0.093417	-3.061687	C	11.066338	1.286584	-2.088091
C	10.335711	-3.349603	-0.541284	C	11.310539	-0.888596	1.858408
C	10.599587	1.708921	0.624979	C	11.358337	-2.240734	-1.574353
C	10.698155	-1.423966	-2.612394	C	11.471247	-1.023488	-2.247251
C	10.824294	0.863477	-2.085169	C	11.50071	1.165239	0.72303
C	11.137171	-1.802832	1.037167	C	11.586336	-2.303808	-0.14069
C	11.204531	-0.44402	1.351684	C	11.816847	0.183346	-1.515484
C	11.24545	-2.233369	-0.346195	C	11.913163	-1.144247	0.564978
C	11.38957	0.53915	0.294152	C	12.030717	0.125588	-0.136977
C	11.422964	-1.290871	-1.359949	C	-10.181269	-3.114416	1.887582
C	11.499524	0.122921	-1.034123	C	-10.404344	0.960558	2.44483
C	-10.071292	-1.761543	-3.132023	C	-10.43886	1.858928	-1.571386
C	-10.264843	-0.11481	2.40577	C	-10.527379	-3.509126	0.59374
C	-10.340177	1.882836	0.959779	C	-10.707328	-1.872075	2.434425
C	-10.44558	-2.654161	-2.125807	C	-10.739949	0.754795	-2.371098
C	-10.486833	-0.368337	-3.059973	C	-10.908897	1.907603	-0.196248
C	-10.730033	-2.192533	1.407858	C	-10.944565	-2.727807	-1.583695
C	-10.78172	-2.874004	0.190306	C	-10.997917	-1.582333	-2.38035
C	-10.976513	1.357864	-1.36701	C	-11.402561	0.367977	1.66918
C	-11.145564	-0.799246	1.479814	C	-11.40844	-2.676716	-0.207824

C	-11.184065	1.221741	0.065723	C	-11.523828	-0.339906	-1.833594
C	-11.245201	-2.190143	-1.004734	C	-11.557576	-1.075774	1.664534
C	-11.259414	0.074626	-1.984728	C	-11.660276	0.851426	0.322228
C	-11.595853	-0.145327	0.331322	C	-11.912653	-1.485629	0.316324
C	-11.643673	-0.85458	-0.935735	C	-11.974852	-0.294264	-0.51291
H	0.157121	2.515392	-2.972243	H	0.833603	-0.221712	1.256784
H	0.402315	0.700439	-0.220881	H	1.233904	1.070818	-0.00376
H	1.08299	1.955657	2.146887	H	1.286812	-4.018432	4.504253
H	1.274054	-2.450583	4.600295	H	1.404091	-3.535616	2.068443
H	1.361135	3.328946	1.08217	H	1.547116	1.039609	3.149782
H	1.729166	-1.867028	2.240815	H	1.729682	2.643348	2.231622
H	1.924355	-0.88548	6.422168	H	2.060469	4.070576	-2.154596
H	2.347377	-0.333691	0.627407	H	2.226669	6.402933	-1.305771
H	2.66465	1.336182	-1.179924	H	2.470168	-2.534739	6.113483
H	2.811822	2.813393	-2.965583	H	2.696929	-1.605943	1.244143
H	2.83841	5.144243	-3.808548	H	3.013499	2.204441	-0.855085
H	3.032299	1.268407	5.857102	H	3.355793	6.845822	0.866891
H	3.323831	7.024229	-2.251864	H	3.744282	-0.584811	5.292316
H	3.503255	1.840884	3.492738	H	4.289917	4.974372	2.180523
H	3.781815	4.214454	0.975645	H	4.513969	0.721032	3.682006
H	3.79942	6.549327	0.141929	H	4.708821	2.822632	2.519207
H	-0.268268	-4.189188	0.11004	H	-0.041366	3.265129	0.199451
H	-0.401256	4.428555	-1.381599	H	-0.5347	-3.101503	-2.172434
H	-0.468524	-4.614762	2.552522	H	-0.658402	-2.325644	-4.532078
H	-0.680865	1.090617	-2.337398	H	-1.177807	1.928613	-1.521405
H	-0.703024	0.584565	1.896385	H	-1.485877	3.331356	1.209333
H	-1.215801	2.36926	1.91523	H	-1.666131	-1.814825	-0.383068
H	-1.298374	-2.172373	-0.88405	H	-1.888752	3.513165	-1.206317
H	-1.553389	2.629595	-2.536548	H	-1.928269	-0.26032	-5.085199

H	-1.692236	-2.995677	3.991333	H	-1.953514	1.533361	2.402526
H	-2.343646	-0.156963	-0.688323	H	-2.716425	0.100272	0.3512
H	-2.732	-0.990062	2.999717	H	-3.074773	1.01155	-3.294094
H	-3.074647	2.300712	-0.552619	H	-3.629519	2.243704	1.295055
H	-3.41975	4.569298	-0.504129	H	-4.223159	4.236765	2.287386
H	-3.605642	6.699014	0.742392	H	-4.323843	3.954427	-1.998708
H	-3.65688	2.383658	3.195246	H	-4.637003	6.67209	2.143022
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N	2.701811	1.744312	0.894271	N	3.315336	1.354606	2.134427
N	-2.485192	1.049931	0.989027	N	-3.084492	1.893582	-0.721931
O	-0.177087	3.896562	-0.598965	O	-1.161371	0.989104	2.241466
<b>3aa</b>				<b>4aa</b>			
C	0.103583	2.74534	0.874755	C	0.110093	-0.797547	-3.80282
C	0.161484	-1.559804	-2.227619	C	0.467821	-0.049009	-4.924127
C	0.593525	-1.323633	0.51276	C	0.514274	4.505712	-0.813395
C	0.847269	2.574203	-0.480487	C	0.597686	-0.44354	-2.543123
C	0.858989	3.665416	1.838784	C	0.657289	2.976663	-0.670567
C	1.011308	-0.567676	-1.738775	C	1.312219	1.054686	-4.778865
C	1.049141	3.194923	3.26837	C	1.452914	0.653757	-2.389259
C	1.239376	-0.440765	-0.36065	C	1.803087	1.403314	-3.521555
C	2.202633	0.594718	0.18637	C	1.990082	1.001159	-1.014839
C	3.310339	2.648074	-0.057788	C	2.785867	2.566553	0.514508
C	3.430433	3.877922	-2.282791	C	3.077885	4.403357	2.216943
C	3.576828	3.888796	-0.88825	C	3.195071	3.977754	0.88907
C	3.715456	5.017466	-3.033663	C	3.433221	-0.955402	-0.203752
C	3.732005	0.179567	0.112524	C	3.452278	0.490001	-0.713992

C	4.005026	5.06504	-0.263526	C	3.481945	5.686029	2.595958
C	4.05708	-0.84849	-0.981557	C	3.610865	-1.310504	1.115858
C	4.146762	-0.619959	1.353274	C	3.726917	4.864562	-0.059061
C	4.157429	6.182634	-2.402351	C	3.852284	-1.858217	-1.239581
C	4.19711	-2.159143	-0.404608	C	4.002193	1.562496	0.346674
C	4.249515	-2.018167	1.037877	C	4.006023	6.561215	1.645066
C	4.300294	6.203803	-1.014961	C	4.119671	-0.322651	2.093794
C	4.489641	1.58591	-0.055791	C	4.124885	6.146518	0.315479
C	4.731095	-0.557635	-2.146265	C	4.185303	-2.594849	1.453119
C	4.89638	-0.104633	2.389012	C	4.336861	0.317297	-1.958388
C	4.945791	-3.159232	-1.034254	C	4.383795	-3.116293	-0.934527
C	5.049129	-2.878202	1.799317	C	4.413697	-1.072843	-2.321704
C	5.411791	1.661443	-1.281455	C	4.417582	0.96339	1.696323
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C	5.503339	1.893949	1.052087	C	4.99459	-1.025313	3.007559
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C	5.751887	-0.971091	3.170967	C	5.48831	-1.576491	-3.062385
C	5.791434	-4.040652	-0.24503	C	5.512833	-3.629747	-1.692851
C	5.821081	-2.340759	2.892964	C	5.625336	1.582699	2.169256
C	5.841718	-3.904481	1.141537	C	5.795606	-4.240586	0.55871
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C	6.644714	0.490458	-3.046993	C	6.053417	-2.875382	-2.733061
C	6.684452	2.495805	0.497725	C	6.147662	-0.407521	3.504115
C	6.711924	-0.925966	-3.356428	C	6.186697	2.362792	1.083313
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C	6.912234	-3.541927	-2.24947	C	6.388784	-4.32549	-0.766393
C	6.961847	-0.240123	3.501988	C	6.470786	0.931014	3.074464

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C	8.005395	1.709232	2.408748	C	7.574669	2.467592	0.944577
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C	8.191049	-0.898446	3.542056	C	7.77408	-4.237706	-0.917698
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C	-0.253683	-2.321573	0.024909	C	9.603326	-2.161746	2.132463
C	-0.471626	-2.441998	-1.347652	C	9.711183	-3.173597	-0.116344
C	-1.298179	3.434991	0.648419	C	9.772436	0.767123	-1.289189
C	-1.881678	2.734746	-4.360189	C	9.839562	-1.496681	-1.921883

C	-1.93663	2.038806	-3.150821	C	-0.964029	4.845868	-0.989413
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C	-2.518049	1.720641	4.080693	C	-2.504291	3.127795	3.508918
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C	-2.660369	2.301575	5.343435	C	-2.911526	-0.363515	0.182392
C	-2.837134	1.70814	1.579945	C	-2.960733	-2.486704	-0.82409
C	-2.968119	2.382061	2.931488	C	-3.064843	-2.356083	1.637501
C	-3.033103	4.591996	-3.336226	C	-3.266082	5.265717	0.183749
C	-3.096374	3.891974	-2.131997	C	-3.306058	-0.19782	-1.234626
C	-3.247499	3.560749	5.469489	C	-3.331104	-1.513528	-1.836496
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C	-4.799104	-0.246136	-2.43517	C	-4.246011	0.745987	-1.588441
C	-5.018672	-3.507264	-0.005969	C	-4.300045	-1.83991	-2.792289
C	-5.202389	1.722417	-1.234284	C	-4.306061	1.68425	0.875726
C	-5.23134	-2.656778	-2.311772	C	-4.447962	4.004028	-3.450918
C	-5.242966	-0.470578	2.698059	C	-4.586182	-4.073593	-1.785195
C	-5.374842	-1.393514	-2.992972	C	-4.594856	4.250777	3.082698
C	-5.450555	1.596714	1.619253	C	-4.641353	4.665806	4.412925
C	-5.526493	1.008373	-2.440339	C	-4.697143	-2.319743	3.325083



C	-5.629707	-2.858313	2.293862	C	-4.72045	-3.634634	2.708655
C	-5.897624	-1.657526	3.046779	C	-4.733697	1.86565	-0.662333
C	-5.970499	0.783949	2.685967	C	-4.864966	4.034857	-2.115546
C	-6.193149	2.430648	-0.59224	C	-4.943707	-3.140532	-2.761054
C	-6.209436	-4.221271	-0.140213	C	-5.129588	0.454447	2.814691
C	-6.32109	2.365541	0.880288	C	-5.171013	4.675182	-4.438648
C	-6.477981	-3.387562	-2.449084	C	-5.219223	-5.022403	0.271425
C	-6.711134	-1.331427	-3.562706	C	-5.26789	0.399335	-2.537277
C	-6.804094	1.071161	-3.006385	C	-5.292944	-0.85736	-3.152813
C	-6.876101	-3.588821	2.151788	C	-5.48078	1.449364	1.836412
C	-6.958629	-4.153608	-1.384929	C	-5.607991	-4.85994	-1.122189
C	-7.161492	-4.256269	0.958782	C	-5.88761	-1.714359	3.724998
C	-7.31228	-1.634777	3.382169	C	-5.93697	-4.29263	2.516381
C	-7.326565	0.807512	3.028081	C	-6.011766	4.770001	-1.782351
C	-7.39507	-2.567226	-3.224233	C	-6.105868	-0.298194	3.476021
C	-7.410196	-0.125279	-3.568471	C	-6.191103	-5.000524	1.274188
C	-7.53009	2.485862	-1.143375	C	-6.245988	1.767761	-0.908976
C	-7.732892	2.38315	1.197026	C	-6.3142	5.399251	-4.099151
C	-7.834246	1.830126	-2.340955	C	-6.343642	-2.956264	-3.109518
C	-7.918679	-2.831448	2.825788	C	-6.504572	1.028372	-2.115861
C	-8.011055	-0.428459	3.372304	C	-6.560137	-1.541064	-3.353885
C	-8.232801	1.628667	2.263571	C	-6.72897	5.44972	-2.766186
C	-8.370146	-4.134837	-1.05484	C	-6.805488	1.613972	1.499434
C	-8.479143	2.458104	-0.045482	C	-6.95253	-4.68209	-1.4553
C	-8.495676	-4.198309	0.394274	C	-7.153808	-2.399044	3.530198
C	-8.753929	-2.546496	-2.903398	C	-7.178422	-3.662364	2.936018
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C	-9.086365	1.109331	-2.478252	C	-7.327509	-3.711544	-2.468203
C	-9.202591	-2.772855	2.2798	C	-7.494183	-0.10776	3.135002

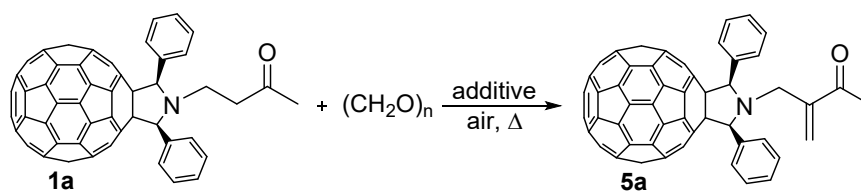
C	-9.25105	-3.345953	-1.797874	C	-7.58916	-4.81002	0.926018
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C	-9.484691	0.908409	2.121698	C	-7.830876	0.826119	2.149323
C	-9.496901	-3.469942	1.040482	C	-7.961748	-4.653917	-0.410068
C	-9.690573	1.778945	-0.179845	C	-8.14823	-1.403061	3.163832
C	-9.932297	-1.515053	2.271596	C	-8.19848	-3.982098	1.95293
C	-9.996722	1.082979	-1.419448	C	-8.45839	1.088081	-0.10167
C	10.00286	-1.736683	-2.24519	C	-8.56908	-3.081461	-2.048499
C	10.170101	-1.278502	2.337036	C	-8.729648	0.408309	-1.293784
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C	10.693927	0.197156	-0.877883	C	-8.849376	0.502122	1.167315
C	10.747033	0.341846	0.56816	C	-8.960094	-3.663875	-0.776829
C	10.757109	-1.219894	-1.189509	C	-9.126517	-1.712453	2.216462
C	10.842355	-0.985949	1.148328	C	-9.153208	-3.025255	1.601589
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C	-10.28878	-2.584402	-1.123113	C	-9.542032	-2.862762	0.208052
C	-10.409145	-2.645098	0.266188	C	-9.755516	-1.449782	-0.037138
C	-10.431231	-1.312674	-1.811378	C	10.129968	0.021246	1.436776
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H	0.077311	2.970698	3.726059	H	0.084968	-0.317916	-5.904895
H	0.184142	2.040528	-1.165425	H	0.105578	2.5268	-1.499748
H	0.763945	-1.237023	1.583806	H	0.167802	2.638077	0.264123
H	1.009432	3.569238	-0.90206	H	0.306311	-1.023527	-1.670383
H	1.508527	0.115778	-2.419889	H	0.931569	5.027797	0.050414
H	1.560703	3.964936	3.849626	H	1.047428	4.825399	-1.713543

H	1.63361	2.266117	3.293553	H	1.341262	0.503701	-0.268447
H	1.986768	0.71062	1.264931	H	1.587111	1.647751	-5.64704
H	3.084369	2.972812	-2.771795	H	2.176541	2.16369	1.346996
H	3.205448	2.966429	0.992884	H	2.450135	2.266802	-3.405441
H	3.593484	4.995332	-4.113481	H	2.666451	3.725754	2.961778
H	4.090621	5.09564	0.819072	H	3.382612	5.999096	3.631793
H	4.380959	7.070138	-2.988432	H	3.810339	4.546435	-1.092959
H	4.629419	7.109609	-0.51305	H	4.318377	7.560672	1.935371
H	-0.001518	-1.650095	-3.29852	H	4.52959	6.824084	-0.431657
H	-0.04983	1.769214	1.34769	H	-0.559254	-1.647489	-3.901576
H	-0.744874	-2.99929	0.717569	H	-1.352357	4.72857	1.126518
H	-1.134658	-3.212874	-1.729563	H	-1.413139	6.322516	0.44317
H	-1.218373	4.08915	-0.223716	H	-1.666907	2.528084	3.158184
H	-1.406185	2.278278	-5.224198	H	-1.754611	3.251869	5.524442
H	-1.500537	4.09101	1.49867	H	-2.417532	2.717742	0.962324
H	-1.502312	1.044419	-3.0778	H	-3.104092	3.020623	-1.493719
H	-1.864748	1.014973	-0.77825	H	-3.542286	3.465365	-3.714685
H	-2.057989	0.739275	3.987315	H	-3.587785	5.784757	-0.721633
H	-2.08239	0.905857	1.678614	H	-3.630993	5.845578	1.03805
H	-2.30895	1.771215	6.224367	H	-3.660981	4.629537	6.335686
H	-2.381108	4.560922	-5.393334	H	-4.83257	4.640977	-5.470782
H	-3.354227	4.018225	6.44921	H	-5.38664	4.525323	2.392632
H	-3.458716	5.589786	-3.401437	H	-5.476184	5.269107	4.759716
H	-3.571228	4.338584	-1.264031	H	-6.331752	4.810664	-0.745922
H	-3.915289	4.163803	2.184793	H	-6.874867	5.927277	-4.86601
H	-4.152022	5.213283	4.418608	H	-7.614059	6.018026	-2.49198
N	2.144906	1.879558	-0.498687	N	2.030594	2.447595	-0.739309
N	-2.49506	2.606972	0.480537	N	-3.959058	3.965338	0.20964
O	1.232437	4.766324	1.470553	O	-1.494697	4.764673	-2.083302

TsOH				TsO <sup>-</sup>			
C	0.121051	-0.005973	-0.078408	C	0.539155	1.203746	-0.035723
C	-0.557007	1.212827	-0.093257	C	0.539155	-1.203729	-0.035724
C	-0.569363	-1.219069	-0.032051	C	1.934298	-1.201161	-0.020992
C	-1.95005	1.209477	-0.051253	C	1.934302	1.201172	-0.020991
C	-1.960267	-1.200058	0.012849	C	2.656197	0.000005	-0.006346
C	-2.671803	0.009658	0.008817	C	4.168072	-0.00001	0.043341
C	-4.179885	0.01336	0.08055	C	-0.16882	0.000011	-0.036744
H	2.776993	0.721452	1.678866	H	2.475018	-2.147606	-0.028159
H	-0.001872	2.14263	-0.156842	H	2.475028	2.147611	-0.028159
H	-0.022987	-2.156007	-0.046955	H	4.543254	-0.000463	1.077409
H	-2.485164	2.155372	-0.072182	H	4.587166	0.886237	-0.448476
H	-2.504215	-2.140849	0.043948	H	4.587205	-0.885814	-0.44925
H	-4.523793	-0.15685	1.109196	H	-0.020158	-2.13372	-0.070202
H	-4.595481	0.969701	-0.251163	H	-0.020167	2.133733	-0.070192
H	-4.611711	-0.779628	-0.539529	O	-2.311673	-0.00016	1.463596
O	2.283669	-0.095873	1.476859	O	-2.366595	-1.253695	-0.698831
O	2.34613	-1.26542	-0.730117	O	-2.366619	1.253834	-0.698569
O	2.386123	1.284432	-0.595902	S	-1.99265	-0.000001	0.010409
S	1.9028	-0.016392	-0.128471				

## Control experiments for mechanistic study

Table S4 Control experiments for mechanistic study<sup>a,b</sup>



Entry	Additive	Molar ratio <sup>b</sup>	Temp. (°C)	Time. ( min )	Yield (%) of <b>5a</b>
1	TsOH·H <sub>2</sub> O	1:10:3	40	360	none
2	TsOH·H <sub>2</sub> O	1:7:2	40	180	none

<sup>a</sup>Unless otherwise indicated, all reactions were performed in chlorobenzene (10 mL) under air conditions. <sup>b</sup>Molar ratio refers to **1a**/(CH<sub>2</sub>O)/TsOH·H<sub>2</sub>O.

## Experimental procedures and spectral data for compounds **1a-l** and **2a-e**

### General procedure for the preparation of ketone-containing fulleropyrrolidines **1**

*N*-unsubstituted fulleropyrrolidines **2** (0.022 mmol), paraformaldehyde (3.3 mg, 0.110 mmol), ketones (0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) were added to a 50 mL round-bottom flask equipped with a reflux condenser and a magnetic stirrer. After they were completely dissolved in chlorobenzene (6 mL) by sonication, the resulting solution was put into an oil bath preset at 80 °C and stirred under air conditions. Thin-layer chromatography (TLC) was employed to carefully monitor the reaction and to stop the reaction at the designated time. The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent evaporation in vacuo was completed, the residue was separated on a silica gel column with carbon disulfide/dichloromethane as the eluent to afford ketone-containing fulleropyrrolidines **1**.

**Ketone-containing fulleropyrrolidine 1a.** According to the general procedure, the reaction of **2a** (20.0 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), acetone (8

$\mu\text{L}$ , 0.110 mmol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 15 min afforded **1a**<sup>1</sup> (7.3 mg, 34%) as amorphous brown solid with  $\text{CS}_2/\text{CH}_2\text{Cl}_2 = 5/2$  as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1b.** According to the general procedure, the reaction of **2b** (21.5 mg, 0.022 mmol) with  $(\text{CH}_2\text{O})_n$  (3.3 mg, 0.110 mmol), acetone (8  $\mu\text{L}$ , 0.110 mmol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1b** (7.7 mg, 33%) as amorphous brown solid with  $\text{CS}_2/\text{CH}_2\text{Cl}_2 = 1/1$  as the eluent: mp > 300 °C; **1b**: <sup>1</sup>H NMR (600 MHz,  $\text{CS}_2/\text{DMSO}-d_6$ )  $\delta$  7.99 (d,  $J = 8.6$  Hz, 2H), 7.48 (d,  $J = 8.3$  Hz, 2H), 6.95 (dd,  $J = 8.6, 2.5$  Hz, 2H), 6.80 (dd,  $J = 8.3, 2.5$  Hz, 2H), 5.39 (s, 2H), 3.75 (s, 6H), 3.26 (t,  $J = 7.7$  Hz, 2H), 2.65 (t,  $J = 7.7$  Hz, 2H), 1.91 (s, 3H); <sup>13</sup>C NMR (150 MHz,  $\text{CS}_2/\text{DMSO}-d_6$ ) (all 2C unless indicated)  $\delta$  203.37 (1C, C=O), 158.48 (aryl C), 153.12, 152.66, 145.94, 145.44, 144.93, 144.84 (4C), 144.75, 144.50, 144.35 (1C), 144.19 (3C), 143.91, 143.86, 143.73, 143.35, 143.04, 141.81 (1C), 141.62 (1C), 141.29, 141.18, 140.87, 140.80, 140.71, 140.67, 140.56, 140.17, 138.61, 138.06, 135.43, 134.34, 130.08 (aryl C), 129.22 (aryl C), 126.97 (aryl C), 114.12 (aryl C), 112.10 (aryl C), 77.79, 73.88, 54.05, 42.47 (1C), 35.99 (1C), 29.40 (1C); FT-IR  $\nu/\text{cm}^{-1}$  (KBr) 2927, 1714, 1609, 1509, 1462, 1429, 1247, 1183, 1170, 1090, 1060, 1032, 944, 889, 857, 829, 799, 713, 685, 627, 570, 528; UV-vis ( $\text{CHCl}_3$ )  $\lambda_{\text{max}}/\text{nm}$  257, 309, 431; HRMS (MALDI-TOF)  $m/z$ :  $[\text{M}]^-$  Calcd for  $\text{C}_{80}\text{H}_{23}\text{NO}_3$  1045.1678; Found 1045.1672.

**Ketone-containing fulleropyrrolidine 1c.** According to the general procedure, the reaction of **2c** (20.8 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), acetone (8 μL, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 15 min afforded **1c** (6.2 mg, 28%) as amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 5/2 as the eluent: mp > 300 °C; **1c**: <sup>1</sup>H NMR (700 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) δ 7.99 (d, *J* = 7.7 Hz, 2H), 7.45 (d, *J* = 7.4 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.3 Hz, 2H), 5.43 (s, 2H), 3.28 (t, *J* = 6.4 Hz, 2H), 2.66 (t, *J* = 6.4 Hz, 2H), 2.35 (s, 6H), 1.91 (d, *J* = 2.3 Hz, 3H); <sup>13</sup>C NMR (175 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) (all 2C unless indicated) δ 203.36 (1C, C=O), 153.10, 152.70, 146.07, 145.57, 145.06, 144.98, 144.91, 144.88, 144.63, 144.50 (1C), 144.33 (3C), 144.04, 143.97, 143.87, 143.47, 143.17, 141.95 (1C), 141.76 (1C), 141.42, 141.32, 140.99, 140.93, 140.84, 140.78, 140.66, 140.30, 138.72, 138.16, 137.11, 135.56, 134.49 (aryl C), 132.43 (aryl C), 129.17 (aryl C), 128.97 (aryl C), 128.22 (aryl C), 128.11 (aryl C), 78.20, 73.92, 42.58 (1C), 35.97 (1C), 28.74 (1C), 20.66; FT-IR ν/cm<sup>-1</sup> (KBr) 2920, 2852, 1715, 1507, 1427, 1361, 1272, 1174, 1120, 1031, 822, 678, 573, 525; UV-vis (CHCl<sub>3</sub>) λ<sub>max</sub>/nm 257, 309, 431; HRMS (MALDI-TOF) *m/z*: [M]<sup>-</sup> Calcd for C<sub>80</sub>H<sub>23</sub>NO 1013.1780; Found 1013.1776.

**Ketone-containing fulleropyrrolidine 1d.** According to the general procedure, the reaction of **2d** (21.7 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), acetone (8 μL, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at

80 °C for 20 min afforded **1d** (7.4 mg, 32%) as amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 4/1 as the eluent: mp > 300 °C; **1d**: <sup>1</sup>H NMR (700 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) δ 8.10 (dd, *J* = 8.3, 1.9 Hz, 2H), 7.59 (dd, *J* = 8.1, 2.0 Hz, 2H), 7.43 (dd, *J* = 8.4, 2.0 Hz, 2H), 7.30 (dd, *J* = 8.1, 2.0 Hz, 2H), 5.52 (s, 2H), 3.27 (t, *J* = 7.6 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.95 (s, 3H); <sup>13</sup>C NMR (175 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) (all 2C unless indicated) δ 203.72 (1C, C=O), 152.69, 152.49, 146.51, 145.62, 145.50, 145.41, 145.33, 145.08, 144.91, 144.79 (4C), 144.67 (1C), 144.48, 144.47 (1C), 144.30, 143.85, 143.58, 142.37 (1C), 142.21 (1C), 141.88, 141.75, 141.32 (4C), 141.24, 141.10 (4C), 140.75, 139.22, 138.71, 135.98, 134.99, 134.54 (aryl C), 133.97 (aryl C), 130.80 (aryl C), 130.12 (aryl C), 128.66 (aryl C), 127.88 (aryl C), 77.69, 73.98, 42.91 (1C), 36.19 (1C), 29.46 (1C); FT-IR ν/cm<sup>-1</sup> (KBr) 2920, 2855, 1718, 1489, 1421, 1364, 1278, 1224, 1166, 1093, 1017, 832, 793, 673, 573, 525; UV-vis (CHCl<sub>3</sub>) λ<sub>max</sub>/nm 256, 311, 430; HRMS (MALDI-TOF) *m/z*: [M]<sup>-</sup> Calcd for C<sub>78</sub>H<sub>17</sub>Cl<sub>2</sub>NO 1053.0687; Found 1053.0681.

**Ketone-containing fulleropyrrolidine 1e.** According to the general procedure, the reaction of **2e** (23.1 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), acetone (8 μL, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1e** (6.1 mg, 25%) as amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 5/1 as the eluent: mp > 300 °C; **1e**: <sup>1</sup>H NMR (700 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) δ 8.35 (d, *J* = 8.1 Hz, 2H), 7.83 (d, *J* = 7.8 Hz, 2H), 7.74



(d,  $J = 8.1$  Hz, 2H), 7.62 (d,  $J = 7.9$  Hz, 2H), 5.68 (s, 2H), 3.28 (t,  $J = 7.4$  Hz, 2H), 2.73 (t,  $J = 7.4$  Hz, 2H), 1.95 (s, 3H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CS}_2/\text{DMSO-}d_6$ ) (all 2C unless indicated)  $\delta$  203.64 (1C, C=O), 152.11, 152.06, 146.33, 145.32, 145.28, 145.24, 145.16, 144.90, 144.64, 144.57 (1C), 144.47 (3C), 144.32 (4C), 144.12, 143.63, 143.39, 142.18 (1C), 142.05 (1C), 141.71, 141.56, 141.13, 141.09, 141.04, 140.90, 140.86, 140.58, 140.09 (aryl C), 139.05, 138.53, 135.87, 134.89, 129.88 (aryl C), 129.54 (q,  $J_{\text{C-F}} = 32.0$  Hz, aryl C), 129.11 (aryl C), 124.97 (aryl C), 124.56 (aryl C), 122.95 (q,  $J_{\text{C-F}} = 271.4$  Hz), 77.29, 73.67, 42.46 (1C), 35.73 (1C), 29.02 (1C); FT-IR  $\nu/\text{cm}^{-1}$  (KBr) 2923, 2852, 1721, 1427, 1364, 1319, 1170, 1126, 1066, 1017, 841, 672, 573, 526; UV-vis ( $\text{CHCl}_3$ )  $\lambda_{\text{max}}/\text{nm}$  257, 312, 431; HRMS (MALDI-TOF)  $m/z$ :  $[\text{M}]^-$  Calcd for  $\text{C}_{80}\text{H}_{17}\text{F}_6\text{NO}$  1121.1214; Found 1121.1210.

**Ketone-containing fulleropyrrolidine 1f.** According to the general procedure, the reaction of **2f** (21.5 mg, 0.022 mmol) with  $(\text{CH}_2\text{O})_n$  (3.3 mg, 0.110 mmol), acetophenone (13  $\mu\text{l}$ , 0.110 mol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1f**<sup>1</sup> (21.8 mg, 89%) as amorphous brown solid with  $\text{CS}_2/\text{CH}_2\text{Cl}_2 = 5/2$  as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1g.** According to the general procedure, the reaction of **2a** (20.0 mg, 0.022 mmol) with  $(\text{CH}_2\text{O})_n$  (3.3 mg, 0.110 mmol), 4-methoxyacetophenone (16.5 mg, 0.110 mmol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1g**<sup>1</sup> (15.8 mg, 67%) as

amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 5/1 as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1h.** According to the general procedure, the reaction of **2a** (20.0 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), acetophenone (13 μL, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 15 min afforded **1h**<sup>1</sup> (21.9 mg, 95%) as amorphous brown solid with CS<sub>2</sub> as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1i.** According to the general procedure, the reaction of **2a** (20.0 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), 4-nitroacetophenone (18.2 mg, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 15 min afforded **1i**<sup>1</sup> (23.5 mg, 98%) as amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 5/1 as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1j.** According to the general procedure, the reaction of **2d** (21.6 mg, 0.022 mmol) with (CH<sub>2</sub>O)<sub>n</sub> (3.3 mg, 0.110 mmol), 4-methoxyacetophenone (16.5 mg, 0.110 mmol) and TsOH·H<sub>2</sub>O (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1j** (14.0 mg, 56%) as amorphous brown solid with CS<sub>2</sub>/CH<sub>2</sub>Cl<sub>2</sub> = 5/2 as the eluent: mp > 300 °C; **1j**: <sup>1</sup>H NMR (400 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) δ 8.12 (d, *J* = 8.0 Hz, 2H), 7.66-7.63 (m, 4H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 7.6 Hz, 2H), 6.79 (d, *J* = 8.5 Hz, 2H), 5.67 (s, 2H), 3.81 (s, 3H), 3.41 (t, *J* = 7.5 Hz, 2H), 3.17 (t, *J* = 7.5 Hz, 2H); <sup>13</sup>C NMR (150 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) (all 2C unless indicated) δ 194.43 (1C, C=O), 162.19 (1C, aryl C), 152.50, 152.28, 146.19, 145.37, 145.18, 145.09, 145.01, 144.75, 144.67, 144.48 (3C), 144.37 (1C), 144.16 (4C), 143.98, 143.54, 143.27,

142.05 (1C), 141.90 (1C), 141.56, 141.42, 141.00 (4C), 140.93, 140.80, 140.79, 140.44, 138.90, 138.40, 135.72, 134.77, 134.23 (aryl C), 133.61 (aryl C), 130.66 (aryl C), 129.90 (aryl C), 129.35 (aryl C), 128.63 (1C, aryl C), 128.41 (aryl C), 127.63 (aryl C), 112.75 (aryl C), 76.92, 73.71, 54.50 (1C), 43.29 (1C), 30.83 (1C); FT-IR  $\nu/\text{cm}^{-1}$  (KBr) 1676, 1649, 1627, 1492, 1169, 1012, 834, 777, 748, 697, 570, 526 ; UV-vis ( $\text{CHCl}_3$ )  $\lambda_{\text{max}}/\text{nm}$  258, 313, 430; HRMS (MALDI-TOF)  $m/z$ :  $[\text{M}]^-$  Calcd for  $\text{C}_{84}\text{H}_{21}\text{Cl}_2\text{NO}_2$  1145.0949; Found 1145.0941.

**Ketone-containing fulleropyrrolidine 1k.** According to the general procedure, the reaction of **2d** (21.6 mg, 0.022 mmol) with  $(\text{CH}_2\text{O})_n$  (3.3 mg, 0.110 mmol), acetophenone (13  $\mu\text{l}$ , 0.110 mol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 30 min afforded **1k**<sup>1</sup> (15.6 mg, 64%) as amorphous brown solid with  $\text{CS}_2$  as the eluent: mp > 300 °C.

**Ketone-containing fulleropyrrolidine 1l.** According to the general procedure, the reaction of **2d** (21.6 mg, 0.022 mmol) with  $(\text{CH}_2\text{O})_n$  (3.3 mg, 0.110 mmol), 4-nitroacetophenone (18.2 mg, 0.110 mmmol) and  $\text{TsOH}\cdot\text{H}_2\text{O}$  (12.6 mg, 0.066 mmol) in chlorobenzene (6 mL) at 80 °C for 20 min afforded **1l** (18.5 mg, 72%) as amorphous brown solid with  $\text{CS}_2/\text{CH}_2\text{Cl}_2 = 5/1$  as the eluent: mp > 300 °C; **1l**:  $^1\text{H}$  NMR (400 MHz,  $\text{CS}_2/\text{DMSO}-d_6$ )  $\delta$  8.20 (d,  $J = 8.6$  Hz, 2H), 8.14 (d,  $J = 8.2$  Hz, 2H), 8.05 (d,  $J = 8.6$  Hz, 2H), 7.65 (d,  $J = 7.0$  Hz, 2H), 7.40 (d,  $J = 8.3$  Hz, 2H), 7.29 (d,  $J = 6.7$  Hz, 2H), 5.74 (s, 2H), 3.43 (s, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CS}_2/\text{DMSO}-d_6$ ) (all 2C unless indicated)  $\delta$  195.19 (1C, C=O), 152.30, 152.09, 148.81 (1C, aryl C),

145.95, 145.13, 144.95, 144.86, 144.78, 144.52, 144.42, 144.25 (3C), 144.13 (1C), 143.92 (3C), 143.75, 143.30, 143.03, 141.83 (1C), 141.67 (1C), 141.33, 141.19, 140.76, 140.71, 140.69, 140.56 (4C), 139.69 (1C, aryl C), 138.65, 138.16, 135.49, 134.53, 133.96 (aryl C), 133.38 (aryl C), 130.58 (aryl C), 129.64 (aryl C), 128.40 (aryl C), 128.24 (aryl C), 127.49 (aryl C), 122.60 (aryl C), 76.27, 73.46, 42.10 (1C), 31.31 (1C); FT-IR  $\nu/\text{cm}^{-1}$  (KBr) 1692, 1607, 1527, 1492, 1345, 1091, 1011, 825, 743, 669, 610, 527; UV-vis ( $\text{CHCl}_3$ )  $\lambda_{\text{max}}/\text{nm}$  257, 312, 430; HRMS (MALDI-TOF)  $m/z$ :  $[\text{M}]^-$  Calcd for  $\text{C}_{83}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_3$  1160.0695; Found 1160.0685.

#### **General procedure for the preparation of *N*-unsubstituted fulleropyrrolidines **2****

A mixture of  $\text{C}_{60}$  (36.0 mg, 0.05 mmol), aromatic aldehyde (0.25 mmol), and arylmethylamine (0.25 mmol) was added to a 50 mL round-bottom flask equipped with a reflux condenser and a magnetic stirrer. After the mixed compounds were completely dissolved in *o*-dichlorobenzene (6 mL) by sonication, the resulting solution was heated with stirring in an oil bath preset at 160 °C under air conditions. The subsequent processing steps are the same as those shown in general procedure for the synthesis of ketone-containing fulleropyrrolidines **1**, and afford *N*-unsubstituted fulleropyrrolidines **2** as amorphous brown solids with carbon disulfide as the eluent.

***N*-unsubstituted fulleropyrrolidines **2a**.** According to the general procedure, the reaction of  $\text{C}_{60}$  (36.0 mg, 0.05 mmol) with benzaldehyde (25  $\mu\text{L}$ , 0.25 mmol) and benzylamine (27  $\mu\text{L}$ , 0.25 mmol) in *o*-dichlorobenzene (6 mL) at 160 °C for 6 h afforded **2a**<sup>2</sup> (26.0 mg, 57%) as amorphous brown solid with  $\text{CS}_2$  as the eluent:

mp > 300 °C.

***N*-unsubstituted fulleropyrrolidines 2b.** According to the general procedure, the reaction of C<sub>60</sub> (36.0 mg, 0.05 mmol) with 4-methoxybenzaldehyde (30 μL, 0.25 mmol) and 4-methoxybenzylamine (33 μL, 0.25 mmol) in *o*-dichlorobenzene (6 mL) at 160 °C for 17 h afforded **2b**<sup>2</sup> (25.6 mg, 53%) as amorphous brown solid with CS<sub>2</sub> as the eluent: mp > 300 °C.

***N*-unsubstituted fulleropyrrolidines 2c.** According to the general procedure, the reaction of C<sub>60</sub> (36.0 mg, 0.05 mmol) with 4-methylbenzaldehyde (29 μL, 0.25 mmol) and 4-methylbenzylamine (32 μL, 0.25 mmol) in *o*-dichlorobenzene (6 mL) at 160 °C for 4 h afforded **2c** (25.0 mg, 53%) as amorphous brown solid with CS<sub>2</sub> as the eluent: mp > 300 °C; **2c**: <sup>1</sup>H NMR (400 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) δ 7.79 (d, *J*=7.5 Hz, 4H), 7.15 (d, *J* = 7.5 Hz, 4H), 5.83 (s, 2H), 3.99 (s, 1H), 2.33 (s, 3H); <sup>13</sup>C NMR (100 MHz, CS<sub>2</sub>/DMSO-*d*<sub>6</sub>) (all 2C unless indicated) δ 153.04, 152.66, 145.85, 145.78, 145.06, 144.92, 144.88, 144.74, 144.50, 144.47 (1C), 144.26 (1C), 144.16, 143.91, 143.84, 143.79, 143.35, 143.06, 141.81 (1C), 141.67 (1C), 141.31, 141.24, 141.06, 140.89, 140.75 (4C), 140.62, 140.19, 138.64, 138.05, 136.44, 135.72, 134.74 (aryl C), 134.30 (aryl C), 128.24 (4C, aryl C), 127.49 (4C, aryl C), 75.44, 73.74, 20.58; FT-IR ν/cm<sup>-1</sup> (KBr) 3316, 1513, 1382, 1180, 814, 665, 614, 579, 528; UV-vis (CHCl<sub>3</sub>) λ<sub>max</sub>/nm 257, 309, 430; HRMS (MALDI-TOF) *m/z*: [M]<sup>-</sup> Calcd for C<sub>76</sub>H<sub>17</sub>N 943.1361; Found 943.1355.

***N*-unsubstituted fulleropyrrolidines 2d.** According to the general procedure, the

reaction of C<sub>60</sub> (36.0 mg, 0.05 mmol) with 4-chlorobenzaldehyde (35.0 mg, 0.25 mmol) and 4-chlorobenzylamine (31 μL, 0.25 mmol) in *o*-dichlorobenzene (6 mL) at 160 °C for 4 h afforded **2d**<sup>2</sup> (24.7 mg, 52%) as amorphous brown solid with CS<sub>2</sub> as the eluent: mp > 300 °C.

***N*-unsubstituted fulleropyrrolidines 2e.** According to our previous study,<sup>7a</sup> the reaction of C<sub>60</sub> (36.0 mg, 0.05 mmol) with 4-trifluoromethylbenzylamine (143 μL, 1.00 mmol) and Fe(ClO<sub>4</sub>)<sub>3</sub>·xH<sub>2</sub>O (46.0 mg, 0.100 mmol) in chlorobenzene (10 mL) at 120 °C for 24 h afforded **2e**<sup>3</sup> (11.0 mg, 21%) as amorphous brown solid with CS<sub>2</sub> as the eluent: mp > 300 °C.

## Reference

1. C. Huang, G. Huang, H.-J. Wang, F.-B. Li, Z. Wang, Y. Huang, L. Liu and C.-Y. Liu, *Adv. Synth. Catal.*, 2018, **360**, 3732.
2. J.-L. Shi, X.-F. Zhang, H.-J. Wang, F.-B. Li, X.-X. Zhong, C.-X. Liu, L. Liu, C.-Y. Liu, H.-M. Qin and Y.-S. Huang, *J. Org. Chem.*, 2016, **81**, 7662.
3. J.-L. Shi, F.-B. Li, X.-F. Zhang, J. Wu, H.-Y. Zhang, J. Peng, C.-X. Liu, L. Liu, P. Wu and J.-X. Li, *J. Org. Chem.*, 2016, **81**, 1769.

