Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Bingel–Hirsch Reaction Mechanisms on $TiSc_2N@I_h$-C_{80}: Role of the Endohedral Titanium Nitride

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Figure S9. Geometries and relative energies of cycloadducts at the level of B3LYP/6-31G*~Lanl2dz (the most favorable orientation for the inner cluster).

As presented in Figure S1, when a singly bonded product is obtained, there are nine feasible configurations for the bromomalonate group. In order to verify the influence of exohedral group on energetics of products, the most favorable orientational product with different attend fragmentations have been calculated at the level of B3LYP/6-31G* (as shown in Figure S2). It is obvious that those products possess similar relative energies, indicating that the configuration of exohedral group has a weak influence on the energetics of conformers.

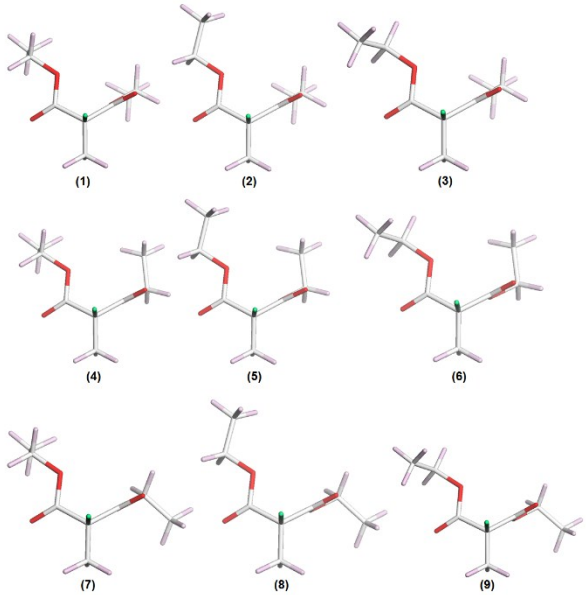

Figure S1. Nine feasible structures of the bromomalonate group considered in this work. The fullerence cage are replaced by one methyl. C, Br, O and H are shown in white, green, red and light pink, respectively.

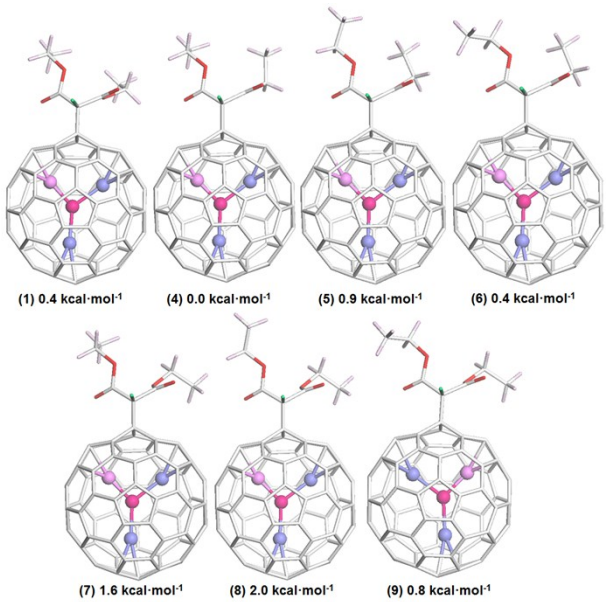

Figure S2. Geometries and relative energies for the most stable 666 products with different attend fragmentations at the level of B3LYP/6-31G*. Two structures with (2), (3) bromomalonate groups cannot be obtained. The numbers in front of relative energies correspond to different attend groups mentioned in Figure S1. Sc, Ti. N are shown in cyan, pink and magenta colors, and Br, O and H are shown in green, red and light pink, respectively.

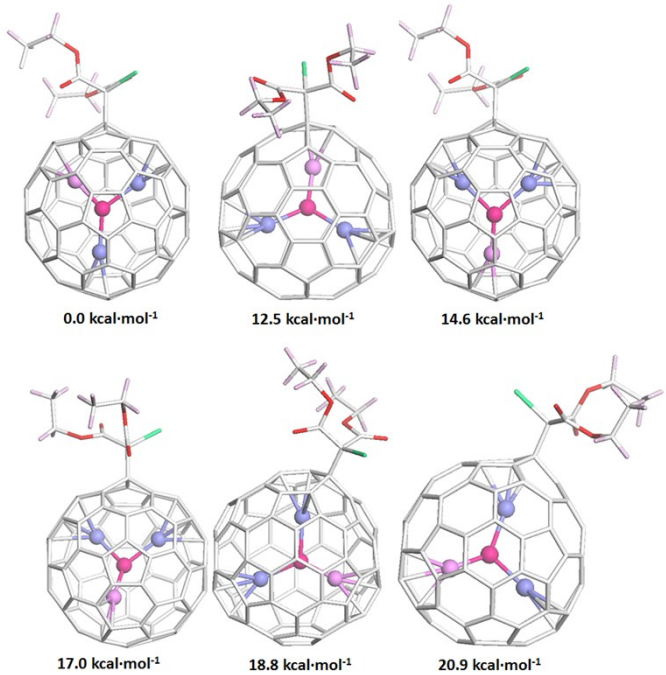

Figure S3. Geometries and relative energies for different orientational 666 products at the level of B3LYP/3-21G.

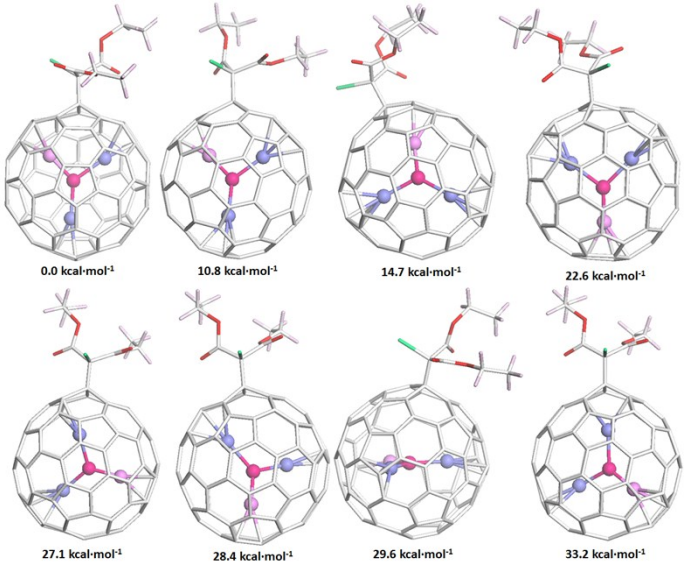

Figure S4. Geometries and relative energies for different orientational 566 products at the level of B3LYP/3-21G.

Table S1. Vertical/Adiabatic electronic affinity (VEA & AEA, in eV) of two singly bonded product.

Singly bonded product	VEA	AEA
666 product	-2.71	-3.02
566 product	-2.54	-2.72

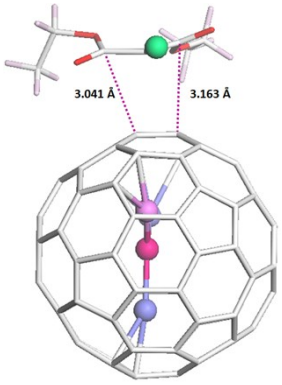

Figure S5. Geometry for transition state of the conversion between 566 and 666 singly bonded products.

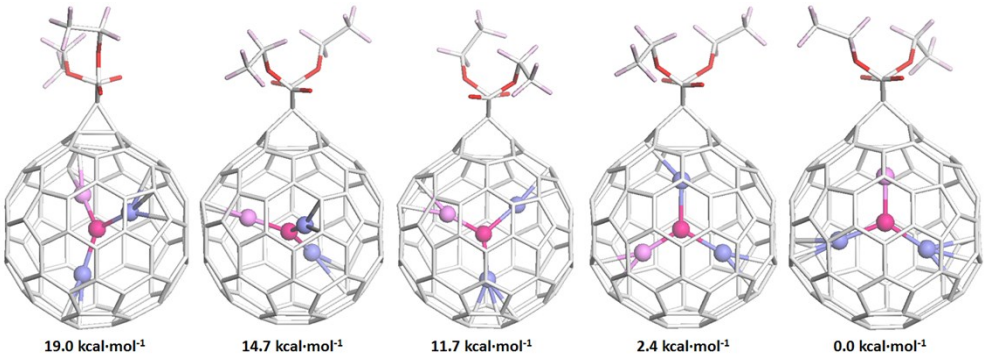

Figure S6. Geometries and relative energies for different orientational [56] cycloadducts at the level of B3LYP/3-21G.

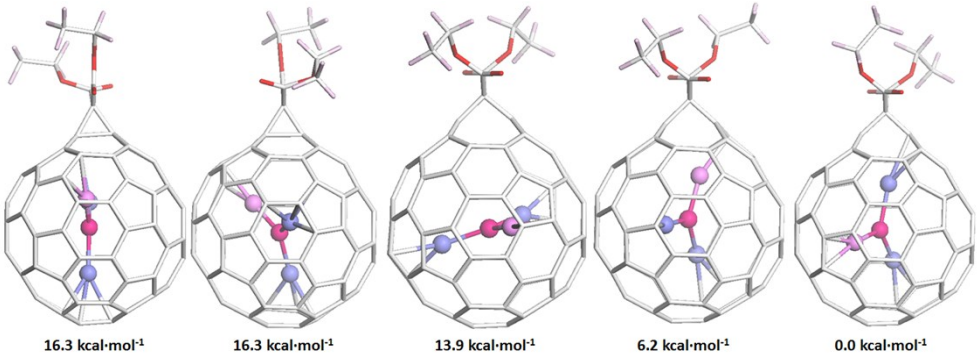

Figure S7. Geometries and relative energies for different orientational [66] cycloadducts at the level of B3LYP/3-21G.

Table S2. Reaction energies (ΔE_r), energy barriers ($\Delta E^{\neq}$) and relative energies (ΔE_{rel}) of intermediates (INT), transition states (TS), and cyclodducts (P) in toluene and gas at the level of B3LYP/6-31G*~Lanl2dz. (Values below are given in kcal·mol^{-1}.)

Phase	P	Bond	INT	E (INT)		E (TS)			E (P)	
		type	/TS	ΔE_r	ΔE_{rel}	ΔE_r	ΔE_{rel}	$\Delta E^{\neq}$	ΔE_r	ΔE_{rel}
Toluene	a	[5,6]	1a	-12.92	3.02	2.61	6.44	15.52	-25.12	0.74
	b	[6,6]	1b	-12.45	3.49	-3.17	0.66	9.27	-25.86	0.00
	b	[6,6]	2b	-15.94	0.00	-3.83	0.00	12.10	-25.86	0.00
Gas	a	[5,6]	1a	-28.26	23.05	-7.87	31.38	20.41	-13.87	6.79
	b	[6,6]	1b	-27.59	23.74	-13.64	25.58	13.94	-13.95	6.71
	b	[6,6]	2b	-31.06	20.27	-14.83	24.39	16.21	-13.95	6.71

Table S3. Reaction energies (ΔE_r), energy barriers ($\Delta E^{\neq}$) and relative energies (ΔE_{rel}) of intermediates (INT), transition states (TS), and cyclodducts (P) in gas at the level of M06-2X/6-31G*~Lanl2dz. (Values below are given in kcal·mol^{-1}.)

P	Bond	INT	E (INT)		E (TS)			E (P)	
	type	/TS	ΔE_r	ΔE_{rel}	ΔE_r	ΔE_{rel}	$\Delta E^{\neq}$	ΔE_r	ΔE_{rel}
a	[5,6]	1a	-48.96	3.15	-19.52	7.97	29.43	-21.85	1.46
b	[6,6]	1b	-48.19	3.91	-23.50	3.98	24.68	-23.31	0.00
b	[6,6]	2b	-52.11	0.00	-27.48	0.00	24.61	-23.31	0.00

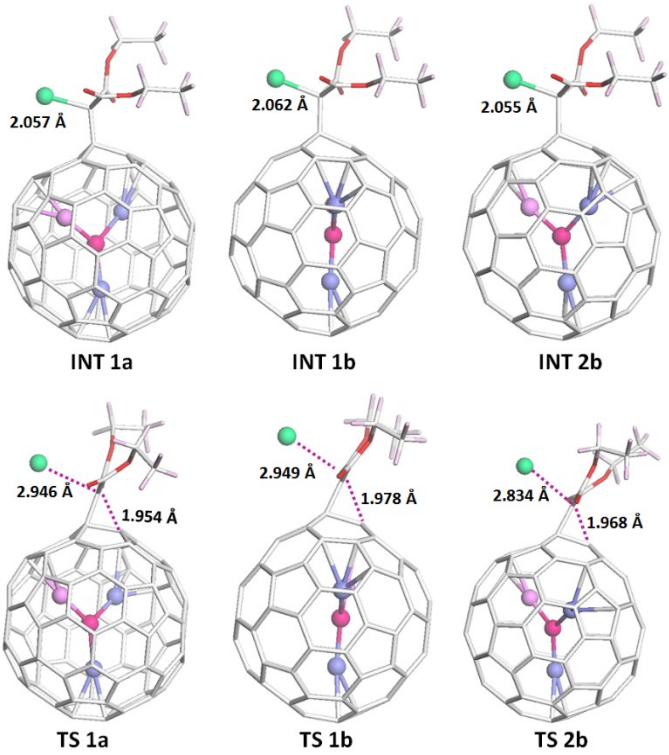

Figure S8. Optimized structures of the intermediates (INT) and transition states (TS).

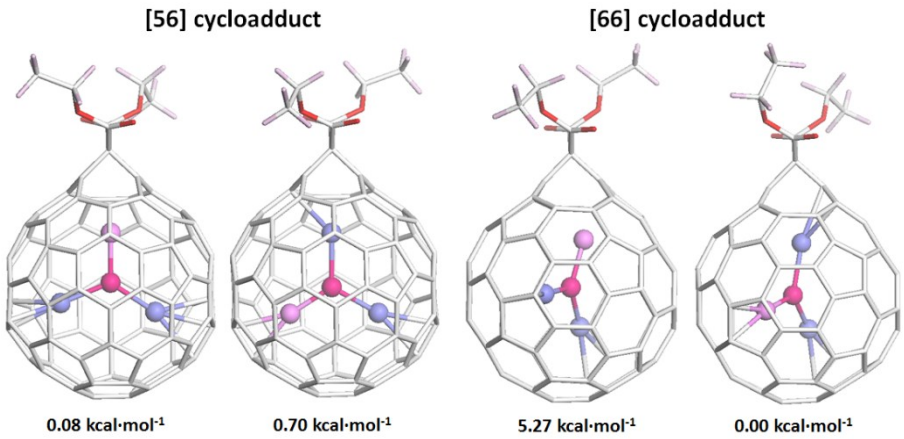

Figure S9. Geometries and relative energies of cycloadducts at the level of B3LYP/6-31G*~Lanl2dz (the most favorable orientation for the inner cluster).

Cartesian coordinates of 666 and 566 singly bonded products.

666 singly bonded product.

C	-2.014386	2.204791	0.630976	C	0.356038	4.608297	-0.606581
C	-1.873715	1.607314	1.918003	C	1.479742	4.586431	-1.482671
C	-1.053909	2.211458	2.937064	C	1.399278	3.765497	-2.676765
C	-0.471966	1.169634	3.722010	C	2.571919	3.046262	-3.169207
C	0.835950	1.329099	4.285553	C	3.845346	3.138588	-2.490054
C	1.652494	0.159742	4.351040	C	4.680474	1.978309	-2.460013
C	3.057139	0.236414	4.190214	C	5.546677	1.714274	-1.345928
C	3.491986	-0.957728	3.490477	C	5.593468	2.589867	-0.214336
C	4.707348	-1.052203	2.731753	C	5.816247	2.011587	1.067481
C	4.683673	-2.025271	1.633175	C	5.176185	2.535312	2.246626
C	5.202321	-1.611432	0.319889	C	4.319481	3.682949	2.193425
C	4.294898	-2.112462	-0.691910	C	3.217460	3.747329	3.096643
C	4.117753	-1.525861	-1.994529	C	1.967710	4.355727	2.718012
C	2.861919	-1.724461	-2.622242	C	1.791034	4.902852	1.416688
C	2.270160	-0.682798	-3.420666	C	2.924140	4.911316	0.543834
C	0.835394	-0.756129	-3.253842	C	2.765987	4.735465	-0.874589
C	0.028720	0.412563	-3.232338	C	3.927683	4.025578	-1.370230
C	-1.140702	0.447529	-2.413438	C	4.799012	3.773713	-0.257504
C	-1.581321	1.664700	-1.771236	C	4.171131	4.312129	0.921464
C	-2.136801	1.326529	-0.491204	C	-1.811684	0.176859	2.080176
C	-1.393299	3.477294	0.431792	C	-0.947915	-0.108156	3.217024
C	-0.821320	3.796944	-0.837048	C	-0.141119	-1.293732	3.271823
C	-0.867117	2.884432	-1.929128	C	1.191037	-1.089950	3.776078
C	0.260993	2.886000	-2.825192	C	2.330308	-1.763673	3.246810
C	0.708062	1.660575	-3.427489	C	2.300772	-2.991425	2.375290
C	2.124014	1.744494	-3.617410	C	3.423111	-2.703905	1.366583
C	2.942031	0.557276	-3.566651	C	3.231180	-2.811137	-0.048648
C	4.252381	0.711479	-3.017240	C	1.961040	-2.981873	-0.673970
C	4.846496	-0.328439	-2.244934	C	1.792532	-2.437460	-1.963581
C	5.645867	0.286893	-1.204976	C	0.540222	-1.848194	-2.369048
C	5.796177	-0.305237	0.084466	C	-0.558420	-1.763564	-1.466550
C	5.893400	0.581887	1.209112	C	-1.428668	-0.641032	-1.534668
C	5.334114	0.222316	2.501741	C	-2.043103	-0.101494	-0.336622
C	4.874854	1.448484	3.122986	C	-1.870593	-0.705762	0.945506
C	3.715252	1.480835	3.964836	C	-1.100290	-1.931902	1.014287
C	2.924426	2.656422	3.984128	C	-0.241618	-2.246186	2.164561
C	1.490391	2.580104	4.138258	C	0.960927	-2.848149	1.633549
C	0.900434	3.629523	3.354216	C	0.840941	-2.951338	0.218343
C	-0.360748	3.445717	2.711451	C	-0.408403	-2.375735	-0.173325
C	-0.572432	4.084100	1.453448	N	2.119406	0.648877	0.292768
C	0.499296	4.788929	0.815502	Sc	0.552955	-0.328083	1.306856

Sc	1.999791	2.196943	-1.106648	Br	4.206602	-4.439038	4.147957
Ti	3.555475	-0.316430	1.017891	C	2.412979	-4.360472	3.168751
C	-2.092233	-5.664474	3.784248	H	-2.323990	-5.040307	2.915377
C	-0.954077	-5.069106	4.588961	H	-2.987929	-5.729893	4.411364
C	1.306674	-4.441145	4.246303	H	-1.843462	-6.671055	3.433436
C	0.964311	-8.377876	1.816904	H	-1.176909	-4.056095	4.935793
C	2.374376	-7.968998	2.212258	H	-0.694773	-5.676637	5.461162
C	2.408727	-5.590635	2.247771	H	0.320775	-8.458569	2.698840
O	0.210690	-5.007831	3.719825	H	0.990609	-9.354002	1.319458
O	1.389346	-4.002362	5.366117	H	0.528668	-7.651501	1.124952
O	2.366816	-6.721487	2.957567	H	2.826012	-8.684286	2.902667
O	2.456734	-5.524875	1.039073	H	3.018145	-7.848110	1.33832

566 singly bonded product.

C	3.015354	-2.051489	-0.861215	C	-2.628192	3.119849	-3.615807
C	2.123206	-2.673927	0.099865	C	-3.563634	2.524976	-2.715431
C	0.976557	-3.378127	-0.452525	C	-4.088311	1.233339	-3.038019
C	-0.160938	-3.112310	0.365663	C	-4.406363	0.276095	-2.013001
C	-1.495007	-3.213161	-0.121808	C	-4.144165	-1.048377	-2.544095
C	-2.431890	-2.300339	0.448556	C	-3.643367	-2.080841	-1.704801
C	-3.518515	-1.761102	-0.302559	C	-2.738690	-3.041290	-2.253155
C	-3.891471	-0.483019	0.282079	C	-1.674826	-3.607785	-1.466184
C	-4.252191	0.586976	-0.624045	C	-0.537070	-3.837920	-2.322734
C	-3.759334	1.900026	-0.304412	C	0.798250	-3.699238	-1.851282
C	-3.430566	2.852536	-1.333705	C	1.804733	-3.220290	-2.736952
C	-2.352660	3.676325	-0.857208	C	1.443373	-2.764717	-4.041210
C	-1.360947	4.197262	-1.746847	C	2.296061	-1.643938	-4.370138
C	-0.028379	4.336482	-1.253189	C	1.841126	-0.566072	-5.193272
C	1.110188	4.131426	-2.107359	C	2.328936	0.742674	-4.883242
C	2.161784	3.541802	-1.320624	C	1.504409	1.921821	-5.052878
C	3.065724	2.594104	-1.883318	C	0.164020	1.835850	-5.547345
C	3.541325	1.539577	-1.040876	C	-0.776968	2.744364	-4.977813
C	3.816066	0.229842	-1.562629	C	-2.160438	2.382390	-4.747071
C	3.483663	-0.732546	-0.543803	C	-2.618086	1.062756	-5.021720
C	2.879904	-2.377933	-2.250669	C	-3.631632	0.507105	-4.191322
C	3.184909	-1.409496	-3.264284	C	-3.660637	-0.902704	-3.883449
C	3.628282	-0.085519	-2.937218	C	-2.672589	-1.798730	-4.391058
C	3.226316	0.984431	-3.787841	C	-2.254102	-2.901826	-3.598543
C	2.947245	2.300576	-3.274383	C	-0.897701	-3.398606	-3.645358
C	1.892737	2.882295	-4.054339	C	0.085437	-2.807446	-4.482262
C	0.934981	3.770292	-3.473603	C	-0.347154	-1.734994	-5.343499
C	-0.400643	3.713021	-3.980102	C	0.519739	-0.659270	-5.777141
C	-1.537775	3.937488	-3.138727	C	-0.312931	0.529034	-5.964189

C	-1.670507	0.156365	-5.622708	Ti	0.995762	-0.890097	-0.429676
C	-1.688802	-1.236980	-5.271996	Sc	-1.830217	0.196719	-0.428871
C	1.662351	-1.947570	1.298456	C	-0.835171	4.418476	5.324597
C	0.229374	-2.172705	1.386152	C	0.263657	3.376029	5.385763
C	-0.716797	-1.233649	1.899771	C	0.546812	1.080716	4.864626
C	-2.074813	-1.352741	1.472123	C	-3.529448	0.907010	7.075618
C	-3.001687	-0.244610	1.424730	C	-2.684883	-0.356057	7.021279
C	-2.434642	1.078655	1.695689	C	-1.569707	-0.330013	4.918194
C	-2.864011	2.132106	0.813678	O	-0.301940	2.118559	4.924209
C	-1.996742	3.226142	0.454023	O	1.705068	1.112042	5.193677
C	-0.644285	3.278552	0.911220	O	-1.477113	-0.148264	6.239960
C	0.323273	3.881556	0.063952	O	-2.579000	-0.636774	4.325208
C	1.678496	3.395490	0.025215	Br	0.841024	-1.814373	4.786987
C	2.076229	2.296894	0.828841	C	-0.197227	-0.132900	4.253002
C	3.047111	1.399135	0.295136	H	-1.198368	4.543448	4.299734
C	3.012385	-0.003978	0.617992	H	-0.446041	5.381490	5.672257
C	2.071335	-0.558462	1.552019	H	-1.680012	4.138208	5.961907
C	1.129160	0.364716	2.088412	H	1.109917	3.625766	4.739283
C	-0.246068	-0.018398	2.670945	H	0.643703	3.226212	6.400601
C	-1.097551	1.170467	2.170028	H	-2.948131	1.747168	7.468843
C	-0.220396	2.231969	1.789059	H	-4.389370	0.744654	7.735313
C	1.132854	1.753018	1.761294	H	-3.903861	1.167928	6.081747
N	-0.195710	-0.167879	-1.694990	H	-2.311881	-0.637607	8.008130
Sc	-0.044618	0.201268	-3.716401	H	-3.238686	-1.192005	6.58807

Cartesian coordinates of transition state for the conversion between 566 and 666 singly bonded products.

C	5.549043	-2.801275	4.663240	C	0.854264	-6.504260	-0.258754
C	5.971817	-4.117963	4.219883	C	-0.205516	-6.444173	0.715306
C	6.224942	-4.264041	2.794506	C	-1.101048	-5.319224	0.784977
C	5.738284	-5.537353	2.363379	C	-1.489492	-5.131515	2.158882
C	5.375596	-5.795858	1.008296	C	-1.788424	-3.831871	2.683008
C	4.286603	-6.704893	0.823015	C	-1.463129	-3.580778	4.047204
C	3.348601	-6.551796	-0.244122	C	-1.013970	-2.284269	4.476609
C	2.085165	-7.155826	0.149709	C	-0.049867	-2.472577	5.529031

C	1.062034	-1.595265	5.677154	C	-0.588231	-0.847713	1.085929
C	2.294905	-2.151033	6.145095	C	-0.644553	-1.767160	-0.032316
C	3.562945	-1.644382	5.691449	C	0.433182	-1.844620	-0.957609
C	4.483311	-2.745776	5.624187	C	0.739980	-3.107346	-1.541523
C	5.664906	-1.693143	3.758112	C	2.098144	-3.479170	-1.856989
C	4.730415	-0.604186	3.810644	C	3.192934	-2.600554	-1.595003
C	3.653294	-0.574732	4.753803	C	4.448611	-3.144583	-1.215631
C	2.427756	0.025571	4.347642	C	5.327696	-2.453152	-0.303990
C	1.154864	-0.476069	4.794348	C	4.978530	-1.198770	0.261246
C	0.199173	-0.295613	3.741994	C	3.738397	-0.604075	-0.171943
C	-0.872720	-1.221127	3.541113	C	2.939601	0.281954	0.650868
C	-1.282930	-1.456702	2.192854	C	1.538996	0.100616	0.262712
C	-1.749933	-2.740450	1.764536	C	1.514536	-0.907205	-0.778505
C	-1.364020	-2.930037	0.385809	C	2.865408	-1.309765	-1.060903
C	-0.985707	-4.212380	-0.111243	C	5.259374	-5.330556	4.660388
C	0.039337	-4.281564	-1.104048	C	5.088401	-6.159588	3.482552
C	0.961375	-5.388186	-1.148382	C	3.984450	-7.068702	3.276183
C	2.236495	-4.882655	-1.623632	C	3.612102	-7.343246	1.917729
C	3.458973	-5.423304	-1.136746	C	2.255245	-7.656564	1.517977
C	4.583772	-4.559192	-0.988295	C	1.202818	-7.523363	2.510283
C	5.530074	-4.741059	0.080627	C	-0.030310	-6.942053	2.072741
C	5.999705	-3.442095	0.501473	C	-0.827079	-6.115011	2.952809
C	6.323239	-3.167232	1.855526	C	-0.426825	-5.832264	4.301320
C	6.083301	-1.864720	2.381608	C	-0.791385	-4.571340	4.848451
C	5.402525	-0.891597	1.590238	C	0.078192	-3.885936	5.768441
C	4.564228	-0.108511	2.470987	C	1.325516	-4.451175	6.147755
C	3.319191	0.449337	2.038120	C	2.418681	-3.557227	6.372066
C	2.263676	0.508218	3.003064	C	3.773381	-3.938116	6.049824
C	0.877525	0.314662	2.627981	C	4.111818	-5.239944	5.557884
C	0.492097	0.066256	1.270868	C	3.000157	-6.115667	5.346294

C	2.955789	-7.051412	4.237535	O	3.066116	-10.211175	6.189124
C	1.581706	-7.249093	3.868611	O	5.210054	-10.668448	2.783636
C	0.777327	-6.445539	4.761033	O	6.609681	-8.951780	3.273289
C	1.644359	-5.763023	5.672561	Br	5.701542	-8.609352	6.229199
N	2.669498	-3.568452	2.248671	C	4.763131	-9.401156	4.713794
Sc	2.160217	-1.694184	1.517715	H	0.781279	-10.743446	2.246688
Ti	3.894967	-4.056407	3.577557	H	0.089014	-12.170003	3.045809
Sc	1.890480	-5.405339	1.600582	H	1.724845	-12.242750	2.353715
C	1.012943	-11.603083	2.885038	H	0.887788	-10.505737	4.763307
C	1.582820	-11.155455	4.219570	H	1.809124	-12.006457	4.869998
C	3.501866	-10.056375	5.060448	H	4.629835	-10.362492	0.167065
C	5.691984	-10.242511	0.406659	H	6.280066	-10.615257	-0.440617
C	6.052854	-11.017653	1.666356	H	5.911402	-9.178908	0.533379
C	5.618618	-9.619146	3.545738	H	5.880853	-12.088809	1.529511
O	2.797892	-10.429884	3.951058	H	7.097116	-10.850128	1.941112

Cartesian coordinates of intermediates (INT), transition states (TS), and cycloadducts.

INT 1a

C	3.018947	-2.052977	-0.857868	C	3.810277	0.236062	-1.537535
C	2.103114	-2.665030	0.071008	C	3.508091	-0.735962	-0.516270
C	0.984486	-3.437837	-0.452257	C	2.889906	-2.375712	-2.249341
C	-0.153301	-3.167932	0.370338	C	3.189670	-1.392950	-3.258454
C	-1.484194	-3.237534	-0.131523	C	3.623190	-0.070513	-2.918586
C	-2.426167	-2.328907	0.441933	C	3.224170	1.006208	-3.764794
C	-3.517324	-1.785951	-0.306620	C	2.943355	2.320010	-3.244266
C	-3.900572	-0.516783	0.289594	C	1.887138	2.903642	-4.022653
C	-4.259148	0.561429	-0.608791	C	0.926215	3.786496	-3.438295
C	-3.768146	1.875524	-0.276965	C	-0.408743	3.729852	-3.948087
C	-3.437950	2.837301	-1.301804	C	-1.546771	3.942259	-3.100950
C	-2.362541	3.660082	-0.819791	C	-2.634206	3.123022	-3.582461
C	-1.370691	4.192540	-1.707369	C	-3.568576	2.518753	-2.686191
C	-0.039938	4.333137	-1.212269	C	-4.092966	1.229230	-3.020474
C	1.099887	4.139377	-2.068533	C	-4.411455	0.262202	-2.003256
C	2.152883	3.547434	-1.283617	C	-4.147115	-1.056955	-2.544753
C	3.056615	2.601888	-1.849601	C	-3.643191	-2.096568	-1.711952
C	3.537082	1.545086	-1.009109	C	-2.734836	-3.047997	-2.265408

C	-1.668631	-3.623613	-1.481208	C	2.076450	2.287728	0.866549
C	-0.531072	-3.839987	-2.334929	C	3.062243	1.398635	0.335965
C	0.809231	-3.714487	-1.849513	C	3.045087	-0.012529	0.653938
C	1.814258	-3.211026	-2.735796	C	2.074578	-0.571539	1.563596
C	1.451557	-2.745920	-4.040833	C	1.131303	0.336954	2.104226
C	2.303408	-1.622916	-4.366463	C	-0.246768	-0.058940	2.674994
C	1.840100	-0.536888	-5.174364	C	-1.100320	1.132391	2.184474
C	2.328140	0.769663	-4.861495	C	-0.222293	2.215396	1.825328
C	1.500470	1.947791	-5.028336	C	1.126663	1.736991	1.785615
C	0.162427	1.863094	-5.530878	N	-0.269851	-0.084277	-1.724012
C	-0.782125	2.766898	-4.952755	Sc	-0.129521	0.250734	-3.701550
C	-2.163265	2.394899	-4.720599	Ti	1.039493	-0.743236	-0.483798
C	-2.620921	1.076254	-5.009195	Sc	-1.853432	0.184524	-0.424372
C	-3.633758	0.513236	-4.180666	C	-0.764088	4.425996	5.142921
C	-3.662926	-0.900429	-3.884303	C	0.306663	3.360373	5.280015
C	-2.668916	-1.788049	-4.395326	C	0.541750	1.039373	4.880972
C	-2.248254	-2.896245	-3.608967	C	-3.560800	0.941099	7.021084
C	-0.888295	-3.386916	-3.652809	C	-2.691706	-0.308143	7.036252
C	0.095595	-2.786516	-4.485451	C	-1.573310	-0.360300	4.938740
C	-0.341551	-1.710618	-5.340728	O	-0.291767	2.095586	4.909544
C	0.520899	-0.627828	-5.762192	O	1.691346	1.065893	5.242749
C	-0.313636	0.558116	-5.961481	O	-1.485576	-0.118072	6.261654
C	-1.674965	0.176800	-5.628110	O	-2.582935	-0.715649	4.377320
C	-1.687099	-1.218357	-5.276408	Br	0.819438	-1.858396	4.821688
C	1.640967	-1.942173	1.265235	C	-0.207098	-0.164737	4.266769
C	0.225428	-2.206780	1.377166	H	-1.120391	4.482097	4.109973
C	-0.720589	-1.282671	1.916163	H	-0.350840	5.402068	5.421178
C	-2.074254	-1.388360	1.473587	H	-1.617573	4.213144	5.795459
C	-3.008629	-0.284414	1.437942	H	1.155228	3.543786	4.614355
C	-2.435244	1.039890	1.712976	H	0.687337	3.278331	6.303325
C	-2.873094	2.102697	0.841467	H	-2.997278	1.809845	7.376909
C	-2.004862	3.200541	0.488257	H	-4.427839	0.797819	7.676876
C	-0.651641	3.256101	0.948579	H	-3.923160	1.145879	6.009917
C	0.314771	3.872652	0.104400	H	-2.329702	-0.534685	8.042246
C	1.667284	3.389029	0.061419	H	-3.231357	-1.172131	6.640697

INT 1b

C	3.123137	-2.081602	-0.963878	C	-4.120826	0.588690	-0.354152
C	2.255234	-2.674588	0.022352	C	-3.605649	1.903333	-0.063715
C	1.102311	-3.440120	-0.434864	C	-3.322860	2.849338	-1.117659
C	0.011992	-3.153784	0.443819	C	-2.217803	3.669505	-0.704928
C	-1.344916	-3.222984	0.016068	C	-1.272314	4.185258	-1.650780
C	-2.249765	-2.301501	0.628555	C	0.083354	4.322817	-1.229243
C	-3.377556	-1.760063	-0.064737	C	1.174121	4.111563	-2.142764
C	-3.720964	-0.482537	0.535656	C	2.262823	3.519488	-1.407550

C	3.129313	2.562702	-2.010817
C	3.646959	1.512555	-1.185269
C	3.882777	0.196650	-1.711828
C	3.629051	-0.762298	-0.664739
C	2.916511	-2.419908	-2.343668
C	3.162833	-1.448253	-3.377116
C	3.622995	-0.124773	-3.077400
C	3.185074	0.944667	-3.913665
C	2.940332	2.265773	-3.394329
C	1.847424	2.847658	-4.121600
C	0.925012	3.744052	-3.497016
C	-0.435452	3.691595	-3.934865
C	-1.524750	3.920493	-3.029757
C	-2.641061	3.102541	-3.441382
C	-3.530123	2.515773	-2.488955
C	-4.079458	1.225889	-2.779048
C	-4.349257	0.273355	-1.734520
C	-4.121136	-1.053796	-2.273506
C	-3.581433	-2.087907	-1.457549
C	-2.708588	-3.050874	-2.047572
C	-1.604667	-3.625178	-1.315249
C	-0.515706	-3.859362	-2.226706
C	0.849679	-3.735400	-1.816953
C	1.809529	-3.252527	-2.762130
C	1.378647	-2.799434	-4.050773
C	2.217813	-1.685113	-4.433980
C	1.718331	-0.605276	-5.228602
C	2.230874	0.701673	-4.958970
C	1.402150	1.883487	-5.093993
C	0.038282	1.801566	-5.522222
C	-0.868009	2.718609	-4.905513
C	-2.236801	2.358215	-4.594572
C	-2.716792	1.039442	-4.841839
C	-3.687322	0.493371	-3.953416
C	-3.708994	-0.916415	-3.639021
C	-2.749804	-1.816498	-4.192411
C	-2.294384	-2.918772	-3.416856
C	-0.941264	-3.419196	-3.528292
C	-0.000072	-2.835817	-4.420261
C	-0.476525	-1.766804	-5.263596
C	0.368725	-0.694449	-5.743410
C	-0.467808	0.494798	-5.910551
C	-1.811545	0.126390	-5.500464
C	-1.813524	-1.264688	-5.132604
C	1.858987	-1.930543	1.228113
C	0.453269	-2.185332	1.417207
C	-0.453878	-1.240488	1.982347
C	-1.832290	-1.347771	1.622728
C	-2.768969	-0.242137	1.638663
C	-2.169455	1.085947	1.862214
C	-2.650202	2.138927	1.002871
C	-1.792533	3.221970	0.587317
C	-0.416494	3.272604	0.973147
C	0.505425	3.874918	0.072091
C	1.848466	3.379786	-0.036802
C	2.292441	2.284485	0.760070
C	3.240553	1.384045	0.184407
C	3.229076	-0.020579	0.520041
C	2.309688	-0.559060	1.491141
C	1.419666	0.363543	2.103818
C	0.055185	-0.017058	2.723429
C	-0.809634	1.173097	2.256988
C	0.053577	2.242163	1.840240
C	1.395338	1.751297	1.739465
N	-0.207107	-0.104207	-1.672579
Sc	-0.164419	0.207998	-3.661089
Ti	1.172757	-0.772586	-0.516434
Sc	-1.705401	0.207619	-0.283309
C	-3.331793	-3.481016	4.681893
C	-3.136362	-2.006205	4.978903
C	-1.409550	-0.391062	4.819085
C	1.024148	-3.992512	6.489819
C	1.515235	-2.578119	6.762921
C	0.955697	-1.312214	4.832093
O	-1.760012	-1.682715	4.667384
O	-2.141279	0.468859	5.241047
O	0.674277	-1.593083	6.119950
O	1.840000	-1.840243	4.199822
Br	0.782866	1.483476	5.224417
C	0.033197	-0.202958	4.305134
H	-3.139640	-3.691062	3.625172
H	-4.363720	-3.770327	4.910632
H	-2.657599	-4.096766	5.286703
H	-3.785071	-1.373846	4.365800
H	-3.318890	-1.764572	6.030989
H	-0.020460	-4.107030	6.797682
H	1.631748	-4.711219	7.052575
H	1.106748	-4.230041	5.425749

H	1.453180	-2.328338	7.825051	H	2.543135	-2.442280	6.417448

INT 2b

C	-2.038184	2.085333	0.590596	C	1.425772	4.573540	-1.485721
C	-1.902000	1.486988	1.879293	C	1.372344	3.761695	-2.691706
C	-1.107235	2.103077	2.907134	C	2.566971	3.048625	-3.143715
C	-0.511807	1.066821	3.697711	C	3.831083	3.159988	-2.450259
C	0.789093	1.249131	4.276167	C	4.704934	2.027834	-2.437025
C	1.624075	0.098392	4.364309	C	5.562552	1.772614	-1.308867
C	3.037527	0.193167	4.235842	C	5.564390	2.641859	-0.168477
C	3.507074	-1.019068	3.600417	C	5.769393	2.056789	1.112820
C	4.667104	-1.010580	2.741259	C	5.115929	2.564393	2.291999
C	4.691053	-1.958773	1.634883	C	4.239493	3.692407	2.230214
C	5.280248	-1.579331	0.336088	C	3.124639	3.722478	3.120709
C	4.399683	-2.098677	-0.690213	C	1.868029	4.311315	2.732871
C	4.209654	-1.489974	-1.983411	C	1.696718	4.862908	1.431716
C	2.964436	-1.716880	-2.632012	C	2.838945	4.902677	0.570185
C	2.357062	-0.677052	-3.424281	C	2.700934	4.732913	-0.853191
C	0.922591	-0.782657	-3.276499	C	3.886449	4.051824	-1.334990
C	0.087691	0.365617	-3.260992	C	4.752215	3.817410	-0.215388
C	-1.090952	0.365525	-2.452561	C	4.096017	4.330407	0.959407
C	-1.565322	1.570319	-1.811348	C	-1.804109	0.054664	2.037880
C	-2.128429	1.212512	-0.538036	C	-0.953617	-0.218184	3.190477
C	-1.440281	3.371591	0.402947	C	-0.116143	-1.391589	3.258360
C	-0.858163	3.710503	-0.858936	C	1.205625	-1.173116	3.794292
C	-0.876831	2.808918	-1.962923	C	2.385126	-1.855654	3.352936
C	0.250072	2.854240	-2.864087	C	2.378542	-3.015007	2.374315
C	0.736119	1.633575	-3.452402	C	3.486784	-2.696617	1.362081
C	2.155431	1.743872	-3.611368	C	3.326872	-2.805080	-0.055016
C	3.003544	0.578550	-3.560488	C	2.067171	-3.004094	-0.696157
C	4.309528	0.758777	-3.002949	C	1.903493	-2.453104	-1.986774
C	4.922454	-0.276010	-2.228555	C	0.642622	-1.887619	-2.398329
C	5.706803	0.346718	-1.181157	C	-0.464618	-1.835744	-1.504886
C	5.846366	-0.257814	0.116466	C	-1.364826	-0.734134	-1.579925
C	5.873707	0.625244	1.246319	C	-2.005397	-0.215002	-0.389267
C	5.290952	0.255667	2.529535	C	-1.823751	-0.817398	0.895032
C	4.828904	1.466396	3.166600	C	-1.023533	-2.022267	0.969354
C	3.663534	1.456574	3.994015	C	-0.174148	-2.320703	2.129565
C	2.843647	2.619706	3.998230	C	1.050125	-2.885755	1.613329
C	1.413217	2.520141	4.145412	C	0.945214	-2.997838	0.190068
C	0.809821	3.559603	3.355972	C	-0.312454	-2.450950	-0.212884
C	-0.438298	3.352884	2.695174	N	2.007865	0.678540	0.234139
C	-0.647368	3.993335	1.435908	Sc	0.580801	-0.351037	1.334524
C	0.414210	4.730221	0.813219	Sc	1.828321	2.205503	-1.086137
C	0.294200	4.554230	-0.612412	Ti	3.568925	-0.258571	0.791599

C	-2.043485	-5.209950	4.026032	C	2.517239	-4.429512	3.109253
C	-0.773451	-4.839936	4.768802	H	-2.249519	-4.487267	3.230698
C	1.524761	-4.529676	4.287248	H	-2.889991	-5.213435	4.722090
C	0.706102	-8.236721	1.617654	H	-1.960083	-6.205698	3.577658
C	2.121413	-8.000561	2.124925	H	-0.834015	-3.841434	5.212204
C	2.407848	-5.641267	2.175305	H	-0.532775	-5.551418	5.565077
O	0.307380	-4.844066	3.805898	H	-0.008630	-8.232770	2.447234
O	1.762633	-4.316392	5.449523	H	0.648589	-9.209581	1.115106
O	2.208521	-6.771448	2.881746	H	0.419877	-7.461147	0.902027
O	2.517361	-5.600085	0.971839	H	2.429481	-8.772926	2.834100
Br	4.402179	-4.621218	3.905770	H	2.837150	-7.957538	1.300291

TS 1a

C	2.944710	-1.767427	-0.570862	C	-4.422876	0.118789	-2.472079
C	1.984430	-2.330463	0.341650	C	-4.062701	-1.232476	-2.871402
C	0.945928	-3.199048	-0.187887	C	-3.600514	-2.178893	-1.907845
C	-0.260431	-2.915178	0.523078	C	-2.622998	-3.141040	-2.304070
C	-1.538717	-3.088314	-0.073204	C	-1.602353	-3.601765	-1.394121
C	-2.554283	-2.167388	0.331900	C	-0.395645	-3.838222	-2.135937
C	-3.623935	-1.749339	-0.527998	C	0.895052	-3.609734	-1.562137
C	-4.099459	-0.438324	-0.084025	C	1.945416	-3.145365	-2.413884
C	-4.439531	0.547918	-1.099614	C	1.669587	-2.814679	-3.780272
C	-3.979581	1.893950	-0.876090	C	2.500458	-1.687789	-4.143752
C	-3.603274	2.775732	-1.949160	C	2.080459	-0.710054	-5.102934
C	-2.598873	3.689268	-1.458771	C	2.490092	0.642952	-4.866912
C	-1.563583	4.180762	-2.322286	C	1.638020	1.768029	-5.203358
C	-0.282023	4.412551	-1.743497	C	0.344814	1.583571	-5.791251
C	0.929763	4.196000	-2.492670	C	-0.674384	2.493783	-5.370080
C	1.940460	3.726518	-1.580993	C	-2.056763	2.092244	-5.214324
C	2.913834	2.768779	-1.980847	C	-2.437892	0.734084	-5.404445
C	3.368898	1.813923	-1.012448	C	-3.491750	0.202245	-4.604968
C	3.730785	0.473762	-1.394239	C	-3.491863	-1.177191	-4.181125
C	3.369706	-0.410720	-0.316139	C	-2.429974	-2.068004	-4.532124
C	2.945343	-2.223559	-1.928458	C	-2.036761	-3.082003	-3.616648
C	3.290902	-1.325399	-2.997751	C	-0.663889	-3.517936	-3.514221
C	3.651255	0.035795	-2.749539	C	0.359001	-2.955247	-4.325318
C	3.278292	1.012628	-3.722562	C	-0.043234	-1.981095	-5.310168
C	2.913732	2.353377	-3.349445	C	0.814373	-0.910092	-5.776293
C	1.906655	2.821550	-4.256781	C	-0.048165	0.224354	-6.125502
C	0.872389	3.713383	-3.829530	C	-1.412271	-0.177413	-5.849139
C	-0.415473	3.557029	-4.431329	C	-1.404985	-1.538140	-5.381599
C	-1.622061	3.800918	-3.697267	C	1.419396	-1.541336	1.442222
C	-2.641357	2.902241	-4.187410	C	0.005792	-1.862372	1.480857
C	-3.613476	2.338809	-3.308136	C	-1.013021	-0.950226	1.867059
C	-4.057936	1.000566	-3.553416	C	-2.292207	-1.119033	1.272641

C	-3.242433	-0.050678	1.045746	C	-2.409286	0.358313	4.368741
C	-2.775995	1.301231	1.253290	O	0.851947	2.087705	4.370777
C	-3.167898	2.258682	0.279889	O	-3.138137	-0.443776	3.809583
C	-2.335003	3.379919	-0.092225	C	-1.153805	0.902176	3.765479
C	-1.024831	3.528436	0.466989	Br	-0.018458	-1.244190	5.433760
C	-0.016766	4.092388	-0.367106	O	-1.143464	2.924221	5.011018
C	1.352240	3.668910	-0.266992	O	-2.673405	0.870077	5.584329
C	1.728554	2.653584	0.648679	C	-0.461674	3.985476	5.711982
C	2.789900	1.766036	0.295944	H	-1.173187	4.299574	6.480643
C	2.793851	0.388545	0.746018	H	0.432127	3.577092	6.190009
C	1.782381	-0.134790	1.639658	C	-3.729399	0.226195	6.322560
C	0.741153	0.767228	1.967538	H	-3.463704	0.395953	7.369357
C	-0.645771	0.378237	2.456555	H	-3.701273	-0.846378	6.116571
C	-1.527968	1.547006	1.959524	C	-0.109451	5.135132	4.777525
C	-0.629745	2.598447	1.469081	H	0.615353	4.810044	4.026721
C	0.707474	2.127661	1.503022	H	-1.003016	5.508247	4.265841
N	-0.314923	-0.028083	-1.869300	H	0.330676	5.960146	5.351048
Sc	0.115220	0.125555	-3.838775	C	-5.091937	0.822524	5.993057
Ti	0.848048	-0.465786	-0.391509	H	-5.091689	1.905752	6.157461
Sc	-2.138659	0.147141	-0.980902	H	-5.354655	0.623908	4.950506
C	-0.357142	1.998980	4.424812	H	-5.860747	0.376416	6.636326

TS 1b

C	3.154640	-2.040221	-1.014642	C	3.651086	-0.025315	-3.079434
C	2.295379	-2.680524	-0.033243	C	3.199611	1.053308	-3.898649
C	1.148141	-3.402859	-0.552977	C	2.917417	2.352825	-3.350157
C	0.035307	-3.167178	0.315665	C	1.826427	2.931295	-4.080787
C	-1.316783	-3.291405	-0.127017	C	0.876777	3.793898	-3.446894
C	-2.241473	-2.394407	0.495768	C	-0.473767	3.728351	-3.912070
C	-3.360925	-1.857700	-0.210601	C	-1.582846	3.918392	-3.023683
C	-3.735919	-0.598939	0.411717	C	-2.675705	3.092221	-3.474333
C	-4.167208	0.483769	-0.455286	C	-3.568116	2.467165	-2.548357
C	-3.676180	1.797581	-0.135419	C	-4.079194	1.171615	-2.873574
C	-3.392594	2.773054	-1.166295	C	-4.339516	0.192262	-1.848804
C	-2.310309	3.601580	-0.717389	C	-4.077013	-1.118767	-2.416091
C	-1.359333	4.153874	-1.632311	C	-3.529803	-2.158422	-1.612090
C	-0.013893	4.303818	-1.181093	C	-2.638487	-3.096488	-2.211009
C	1.096133	4.133514	-2.081101	C	-1.534450	-3.656814	-1.470455
C	2.181757	3.543193	-1.341631	C	-0.424617	-3.853053	-2.375732
C	3.082060	2.622159	-1.955648	C	0.924129	-3.695251	-1.950035
C	3.611209	1.567846	-1.152695	C	1.896603	-3.195619	-2.868819
C	3.883098	0.271921	-1.707602	C	1.474372	-2.720428	-4.150082
C	3.591598	-0.714832	-0.697097	C	2.294755	-1.579731	-4.492094
C	2.982943	-2.353506	-2.409017	C	1.791210	-0.495576	-5.280650
C	3.220836	-1.351978	-3.412964	C	2.269927	0.816928	-4.969558

C	1.419108	1.985681	-5.087950	C	1.345765	0.306916	2.110284
C	0.062923	1.888742	-5.541766	C	-0.020588	-0.111942	2.663457
C	-0.870178	2.769540	-4.912744	C	-0.905505	1.073769	2.259250
C	-2.238867	2.380036	-4.636067	C	-0.067405	2.140403	1.838677
C	-2.685479	1.057940	-4.916799	C	1.300159	1.675614	1.752106
C	-3.659226	0.472980	-4.056894	N	-0.199098	-0.125090	-1.745111
C	-3.652130	-0.943014	-3.769193	Sc	-0.049521	0.259589	-3.733022
C	-2.667100	-1.813688	-4.329383	Ti	1.079705	-0.945856	-0.614120
C	-2.202988	-2.920420	-3.569665	Sc	-1.796979	0.204508	-0.461652
C	-0.839782	-3.394732	-3.675189	C	-1.538708	-0.860108	4.607936
C	0.100854	-2.775729	-4.540647	C	0.983718	-1.667168	4.450551
C	-0.381581	-1.695628	-5.367159	O	-2.421413	-0.078582	4.298667
C	0.450557	-0.599749	-5.819402	O	2.097538	-1.580445	3.960060
C	-0.408923	0.579434	-5.963689	Br	0.576253	0.990294	6.059828
C	-1.746696	0.177217	-5.571645	C	-0.199467	-0.903659	3.936752
C	-1.727271	-1.221394	-5.238664	O	-1.716878	-1.815382	5.538942
C	1.845639	-1.966154	1.177288	O	0.710864	-2.506935	5.464208
C	0.446329	-2.256098	1.347928	C	-2.932783	-1.727772	6.305582
C	-0.511704	-1.421998	2.053289	H	-2.684304	-2.209410	7.255354
C	-1.863487	-1.465683	1.522592	H	-3.165934	-0.675697	6.485410
C	-2.789272	-0.364343	1.510819	C	1.853310	-3.103528	6.107515
C	-2.242783	0.964569	1.786021	H	1.508794	-3.305376	7.125425
C	-2.736334	2.024379	0.951844	H	2.663831	-2.371784	6.141798
C	-1.897629	3.131091	0.574613	C	-4.086673	-2.439296	5.610121
C	-0.533977	3.191240	0.985291	H	-4.330601	-1.938404	4.669507
C	0.391982	3.829721	0.114877	H	-3.828497	-3.483158	5.399593
C	1.746739	3.362698	0.017061	H	-4.976322	-2.427261	6.252092
C	2.194766	2.255872	0.790329	C	2.291123	-4.384446	5.408029
C	3.162060	1.395121	0.201870	H	1.459250	-5.094551	5.342179
C	3.142297	-0.008694	0.491680	H	2.649758	-4.164837	4.398910
C	2.237552	-0.581231	1.439165	H	3.104853	-4.859023	5.970671

TS 2b

C	-1.914766	2.611561	0.225652	C	3.934424	-1.887945	-1.655739
C	-1.892928	2.090154	1.563943	C	2.707575	-2.016255	-2.360485
C	-1.105904	2.696015	2.601412	C	2.284384	-0.977283	-3.266239
C	-0.757354	1.675641	3.561599	C	0.844586	-0.897968	-3.209953
C	0.559724	1.745074	4.165618	C	0.165737	0.343405	-3.329050
C	1.247242	0.510583	4.357759	C	-1.040033	0.551141	-2.596185
C	2.672891	0.421502	4.321776	C	-1.397980	1.855701	-2.088916
C	3.002379	-0.890976	3.816929	C	-2.071832	1.672794	-0.832594
C	4.193575	-1.084488	3.031745	C	-1.161038	3.800848	-0.008360
C	4.160445	-2.118740	2.009805	C	-0.478657	3.969521	-1.253916
C	4.861510	-1.922822	0.728547	C	-0.551782	2.984943	-2.281800
C	3.973772	-2.404145	-0.308818	C	0.625449	2.813090	-3.097903

C	0.980391	1.502065	-3.565914	C	1.696983	-2.790524	2.649293
C	2.408287	1.427934	-3.648994	C	2.891717	-2.724149	1.720460
C	3.093747	0.173956	-3.457286	C	2.781480	-2.899428	0.313104
C	4.379109	0.236452	-2.835560	C	1.534050	-3.029973	-0.395789
C	4.810621	-0.798328	-1.948749	C	1.527131	-2.568796	-1.739779
C	5.597572	-0.189141	-0.895616	C	0.379827	-1.887880	-2.273063
C	5.588158	-0.698131	0.449764	C	-0.759251	-1.639368	-1.453146
C	5.674421	0.262612	1.506113	C	-1.496156	-0.433430	-1.661582
C	4.984693	0.073555	2.771748	C	-2.134189	0.255550	-0.567707
C	4.667737	1.377351	3.297468	C	-2.053971	-0.250058	0.758211
C	3.466226	1.572710	4.041194	C	-1.385144	-1.496006	0.956190
C	2.795337	2.824576	3.901155	C	-0.665189	-1.781445	2.170531
C	1.356829	2.909488	3.958436	C	0.388252	-2.727256	1.834815
C	0.936907	3.960123	3.063544	C	0.358207	-2.908141	0.386912
C	-0.284883	3.849740	2.338643	C	-0.763717	-2.198595	-0.133753
C	-0.352101	4.403246	1.026797	N	1.921089	0.855317	0.382054
C	0.826755	4.949654	0.420337	Sc	0.408866	0.725644	1.771900
C	0.759896	4.676444	-0.995398	Sc	2.110757	2.177398	-1.162295
C	1.929411	4.494584	-1.796686	Ti	3.226088	-0.450854	0.902000
C	1.839724	3.593493	-2.934106	C	0.165507	-4.174609	4.224237
C	2.958875	2.710237	-3.267588	C	1.362964	-5.289105	2.134378
C	4.188534	2.721704	-2.502648	O	-0.155005	-3.198721	4.877717
C	4.895367	1.491248	-2.336423	O	2.340220	-5.389967	1.419610
C	5.651632	1.223787	-1.137068	C	1.095796	-4.111072	3.041363
C	5.708570	2.174925	-0.066498	Br	3.019655	-5.090009	4.878246
C	5.772897	1.677525	1.263393	O	0.365574	-6.191034	2.124742
C	5.134783	2.359288	2.361410	O	-0.297725	-5.409339	4.481416
C	4.412185	3.572811	2.157112	C	-0.990184	-5.572133	5.733774
C	3.260454	3.811238	2.969539	H	-0.833648	-6.623856	5.988091
C	2.112909	4.520416	2.459208	H	-0.507474	-4.946618	6.488414
C	2.078870	4.973066	1.107822	C	0.602986	-7.358225	1.314518
C	3.262122	4.804778	0.321316	H	1.541090	-7.823774	1.632890
C	3.180640	4.544029	-1.093929	H	0.722832	-7.050016	0.270196
C	4.292042	3.684540	-1.447360	C	-2.472930	-5.247095	5.605984
C	5.054841	3.432873	-0.255287	H	-2.613327	-4.188443	5.372285
C	4.412652	4.116867	0.833056	H	-2.934949	-5.848384	4.815213
C	-2.019777	0.686593	1.857777	H	-2.986703	-5.466188	6.550381
C	-1.347142	0.403553	3.121405	C	-0.585833	-8.283644	1.502606
C	-0.584891	-0.831761	3.241243	H	-0.689429	-8.569861	2.554000
C	0.707654	-0.751333	3.882294	H	-1.514160	-7.797045	1.185188
C	1.796184	-1.617426	3.592232	H	-0.449522	-9.192495	0.905156

[56] cycloadduct

C	-3.929765	1.206642	0.496391	C	-2.584419	1.566058	2.572643
C	-3.492077	0.751524	1.792453	C	-1.836319	0.715456	3.443905

C	-0.489349	1.030762	3.807421
C	0.405041	-0.062832	4.007930
C	1.790691	0.037528	3.640608
C	2.222747	-1.258793	3.192761
C	3.219641	-1.412143	2.173364
C	3.103085	-2.561854	1.302382
C	3.378008	-2.384451	-0.104679
C	2.464280	-3.193240	-0.856678
C	2.079160	-2.871318	-2.201052
C	0.759465	-3.236101	-2.584844
C	-0.008463	-2.377767	-3.442292
C	-1.385703	-2.455500	-3.032672
C	-2.243025	-1.324327	-3.108775
C	-3.274335	-1.173180	-2.091934
C	-3.740398	0.164224	-1.729395
C	-4.461326	0.276658	-0.475965
C	-3.323830	2.388960	-0.025296
C	-2.974175	2.480777	-1.418402
C	-3.078805	1.335106	-2.265617
C	-2.132873	1.159665	-3.294745
C	-1.725373	-0.149058	-3.725741
C	-0.350456	-0.068511	-4.139169
C	0.545783	-1.163213	-3.944516
C	1.911262	-0.865040	-3.643570
C	2.672223	-1.712147	-2.773103
C	3.582835	-0.881419	-2.018115
C	3.917013	-1.175178	-0.667806
C	4.154859	-0.103084	0.240155
C	3.772776	-0.214646	1.632313
C	3.358427	1.086232	2.090289
C	2.330444	1.230364	3.070652
C	1.461186	2.357981	2.975189
C	0.066379	2.253933	3.328206
C	-0.685594	3.102773	2.454264
C	-2.008277	2.761803	2.046226
C	-2.404411	3.162441	0.737153
C	-1.477656	3.776003	-0.178984
C	-1.824952	3.337490	-1.516645
C	-0.822172	3.144753	-2.522266
C	-1.005406	2.048166	-3.418219
C	0.095206	1.280485	-3.943080
C	1.430558	1.566146	-3.539614
C	2.349508	0.491399	-3.434654
C	3.381447	0.480437	-2.424157
C	3.517841	1.539589	-1.483444
C	3.967030	1.254173	-0.160531
C	3.476547	1.993562	0.983168
C	2.541127	3.053760	0.838161
C	1.568750	3.249789	1.861946
C	0.239635	3.719184	1.531995
C	-0.130930	4.083086	0.199929
C	0.880150	4.010742	-0.841123
C	0.531523	3.532617	-2.185688
C	1.606999	2.683399	-2.640112
C	2.616392	2.645166	-1.623099
C	2.158803	3.424317	-0.505036
C	-3.294375	-0.654034	2.218562
C	-2.264338	-0.637662	3.236504
C	-1.352486	-1.723742	3.387074
C	-0.022756	-1.415494	3.804082
C	1.100414	-2.168073	3.299109
C	0.942395	-3.279117	2.402855
C	1.982225	-3.490921	1.416664
C	1.587814	-3.848232	0.067086
C	0.234937	-4.160974	-0.318280
C	-0.141332	-3.868685	-1.655474
C	-1.464747	-3.381622	-1.934441
C	-2.407182	-3.216187	-0.898578
C	-3.398064	-2.169381	-1.029332
C	-4.166797	-1.775229	0.134320
C	-3.488866	-1.844122	1.411971
C	-2.551700	-2.908805	1.566100
C	-1.519799	-2.861106	2.543137
C	-0.396039	-3.600488	2.027231
C	-0.751034	-4.089436	0.708910
C	-2.080919	-3.658771	0.423217
N	-0.282048	-0.073847	0.048780
Sc	0.192819	1.835548	-0.645887
Ti	-2.180674	-0.409550	-0.006697
Sc	1.108324	-1.436835	0.848638
C	-5.339042	-0.870810	-0.087743
C	-6.273953	-1.361985	-1.221457
O	-7.030461	-0.346960	-1.657689
C	-7.988640	-0.665226	-2.703486
H	-7.439868	-1.067125	-3.560579
H	-8.654750	-1.449990	-2.332094
C	-6.254394	-0.615350	1.126622
O	-6.645240	-1.784894	1.651917

C	-7.575657	-1.726083	2.769743	H	-9.468107	0.411326	-3.827057
H	-8.102522	-2.681066	2.719917	H	-9.259461	1.001513	-2.164610
H	-8.278459	-0.908843	2.591481	C	-6.841562	-1.554503	4.089792
O	-6.329458	-2.499397	-1.622324	H	-6.327356	-0.590044	4.127897
O	-6.615840	0.477517	1.493846	H	-7.561192	-1.591552	4.915534
C	-8.732168	0.611997	-3.040990	H	-6.109031	-2.354645	4.236145
H	-8.043437	1.382372	-3.401734				

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C	-3.981350	1.078822	0.377960	C	-0.400096	1.530869	3.764732
C	-3.750751	0.466176	1.649372	C	-1.068094	2.568203	3.027572
C	-2.973805	1.094803	2.676836	C	-2.345945	2.351053	2.427547
C	-2.316343	0.057360	3.429948	C	-2.609785	2.992914	1.177916
C	-0.998174	0.249075	3.937990	C	-1.604442	3.776584	0.508680
C	-0.121564	-0.880465	3.961073	C	-1.807487	3.651400	-0.918007
C	1.292142	-0.767331	3.745711	C	-0.696892	3.631829	-1.812491
C	1.770909	-1.969849	3.091920	C	-0.756928	2.819055	-2.976957
C	2.876579	-1.905917	2.151355	C	0.416734	2.180059	-3.521669
C	2.970385	-2.832982	1.015587	C	1.694204	2.338650	-2.917319
C	3.324218	-2.286136	-0.274529	C	2.620700	1.262716	-2.968135
C	2.521770	-2.909509	-1.274577	C	3.539631	1.018931	-1.879665
C	2.258463	-2.274289	-2.523619	C	3.557826	1.828875	-0.713125
C	0.993254	-2.539410	-3.100145	C	3.842497	1.224913	0.550866
C	0.321944	-1.515654	-3.848342	C	3.196030	1.697615	1.754237
C	-1.084181	-1.668247	-3.627759	C	2.342102	2.845040	1.775330
C	-1.932778	-0.527668	-3.589867	C	1.232214	2.781219	2.681754
C	-3.026699	-0.576344	-2.660267	C	-0.063866	3.338924	2.348948
C	-3.550967	0.599305	-2.018342	C	-0.307240	3.951118	1.078012
C	-4.155561	0.204891	-0.764517	C	0.820784	4.084362	0.181364
C	-3.422366	2.378533	0.164561	C	0.602166	3.841018	-1.226275
C	-2.928067	2.790901	-1.130586	C	1.758788	3.189064	-1.762360
C	-2.931627	1.884761	-2.236283	C	2.689235	2.980427	-0.689805
C	-1.876594	1.938796	-3.186630	C	2.140722	3.556101	0.524938
C	-1.386630	0.755730	-3.859404	C	-3.588446	-0.969147	1.781166
C	0.025257	0.909535	-4.067579	C	-2.722343	-1.215161	2.898417
C	0.904676	-0.216509	-4.016407	C	-1.828259	-2.320331	2.867480
C	2.226636	-0.004966	-3.514676	C	-0.542176	-2.139365	3.450220
C	2.895790	-1.031342	-2.768098	C	0.607907	-2.859514	2.977292
C	3.704508	-0.402658	-1.756809	C	0.434514	-3.980389	2.102531
C	3.892375	-0.998074	-0.483241	C	2.111416	-3.967919	0.732596
C	4.016645	-0.184979	0.674844	C	1.645295	-3.856568	-0.637626
C	3.475714	-0.611698	1.950342	C	0.269304	-3.947819	-1.123795
C	2.981587	0.560206	2.615686	C	0.009872	-3.330669	-2.393560
C	1.868264	0.509299	3.495953	C	-1.280197	-2.786787	-2.732831
C	1.013115	1.654332	3.552062	C	-2.335124	-2.815012	-1.793298

C	-3.262957	-1.704879	-1.803841
C	-3.979382	-1.240831	-0.632351
C	-3.632148	-1.826265	0.641031
C	-2.761334	-2.968070	0.644759
C	-1.895132	-3.201875	1.747852
C	-0.739685	-3.919886	1.279290
C	-0.841566	-4.037200	-0.187450
C	-2.122558	-3.472348	-0.544821
N	-0.144474	-0.124483	0.140753
Sc	0.746497	1.758238	0.364262
Ti	-1.978568	-0.266743	-0.378776
Sc	0.767460	-1.965681	0.598111
C	1.565019	-4.899821	1.760279
C	2.538921	-5.195954	2.923044
O	3.615261	-5.831249	2.435838
C	4.648696	-6.204764	3.389673
H	4.166713	-6.504596	4.323014
H	5.129377	-7.070539	2.929616
C	1.111103	-6.268922	1.206334
O	0.446946	-6.927111	2.168199
C	-0.039638	-8.258477	1.839104
H	-0.385291	-8.253137	0.802885
H	-0.890450	-8.398941	2.508637
O	2.344298	-4.928110	4.083612
O	1.334416	-6.682638	0.094738
C	5.629249	-5.063354	3.605755
H	5.132518	-4.206336	4.069774
H	6.435332	-5.393129	4.270898
H	6.073748	-4.746494	2.656901
C	1.037457	-9.307114	2.065617
H	1.401801	-9.274622	3.097500
H	0.623392	-10.304379	1.878727
H	1.879020	-9.153148	1.384156