Supplementary Materials for

The kinetics of uncatalyzed and catalyzed urethane forming reaction of aliphatic diisocyanates with butan-1-ol

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Table S1. Cartesian Coordinates of the N-H-N ring precomplex

Total Energy [Hartree]	Atom	Cartesian Coordinates		
		X	Y	Z
-805.749137	C	-3.57478	-0.92796	-0.84999
	C	-2.9263	-1.68139	0.3277
	C	-1.93547	-2.80645	-0.0351
	C	-0.47318	-2.38685	-0.24721
	C	-1.99751	1.12038	-0.97062
	C	-2.67264	-0.03403	-1.71697
	H	-4.06341	-1.65987	-1.50819
	H	-2.44041	-0.9766	1.01521
	H	-1.9507	-3.56407	0.76163
	H	-0.38344	-1.62252	-1.01835
	H	-1.88351	-0.62215	-2.20084
	H	-2.27346	-3.32586	-0.94236
	H	-3.74636	-2.1299	0.90316
	H	-4.38027	-0.29968	-0.44756
	H	-3.27975	0.38993	-2.52699
	H	-1.32592	0.74641	-0.19104
	H	0.10538	-3.25841	-0.58845
	H	-1.39147	1.70405	-1.67384
	N	0.10628	-1.84579	0.98036
	N	-2.9869	2.00466	-0.37772
	H	-0.00373	-2.39246	1.82544
	C	-3.10911	2.79454	0.52106
	O	-3.36215	3.59035	1.3603
	C	1.09364	-0.9099	1.0819
	O	1.31926	-0.28795	-0.1074
	O	1.6761	-0.64251	2.12183
	C	2.3441	0.73324	-0.10736
	C	3.72985	0.14497	-0.3456
	H	2.30185	1.27861	0.8388
	H	2.05584	1.40591	-0.92083
	C	4.80913	1.23177	-0.442
	H	3.96655	-0.54237	0.4756
	H	3.71154	-0.44734	-1.27054
	C	6.21041	0.6608	-0.67621
	H	4.55848	1.92649	-1.25636
	H	4.80858	1.8271	0.4816
	H	6.96067	1.45869	-0.7276
	H	6.50331	-0.01867	0.13379
	H	6.26002	0.09674	-1.61617

Table S2. Cartesian Coordinates of the N-H-N ring TS

Total Energy [Hartree]	Atom	Cartesian Coordinates		
		X	Y	Z
	C	-3.38694	1.91934	-0.51895
	C	-2.05386	1.53799	-1.19281
	C	-0.76586	2.05728	-0.51622
	C	-0.15602	1.17383	0.58574
	C	-3.78704	-0.20671	0.90254
	C	-3.69093	1.32143	0.86454
	H	-3.42965	3.01387	-0.43269
	H	-1.99996	0.44898	-1.33544
	H	0.00799	2.1968	-1.28129
	H	-0.87196	1.01798	1.40419
	H	-2.93557	1.62645	1.59913
	H	-0.96043	3.0511	-0.08825
	H	-2.08729	1.94857	-2.20967
	H	-4.20375	1.63477	-1.19399
	H	-4.6458	1.73131	1.21723
	H	-2.82623	-0.6625	0.63073
	H	0.71128	1.6755	1.01605
	H	-4.02119	-0.53458	1.92292
	N	0.30579	-0.11411	0.08368
-805.730875	N	-4.81056	-0.68455	-0.00773
	H	-0.34221	-0.71546	-0.40446
	C	-5.36805	-1.71554	-0.29423
	O	-5.98862	-2.64792	-0.66838
	C	1.54444	-0.67291	0.22075
	O	2.39458	0.14458	0.89884
	O	1.84151	-1.77337	-0.21366
	C	3.73809	-0.35539	1.07057
	C	4.61782	-0.04729	-0.13619
	H	3.69396	-1.43133	1.25831
	H	4.10398	0.15361	1.96743
	C	6.0719	-0.48771	0.0801
	H	4.19975	-0.55847	-1.01151
	H	4.57957	1.03161	-0.33927
	C	6.97025	-0.18343	-1.12313
	H	6.47722	0.00909	0.97342
	H	6.09743	-1.56581	0.29095
	H	8.00061	-0.51036	-0.94366
	H	6.60946	-0.69406	-2.02397
	H	6.99354	0.89189	-1.33842

Table S3. Cartesian Coordinates of the N-H-N ring

Total Energy [Hartree]	Atom	Cartesian Coordinates		
		X	Y	Z
	C	-2.44391	0.60619	-0.51075
	C	-0.98897	0.64429	-0.0095
	C	-0.02781	-0.27601	-0.77721
	C	0.23328	0.15497	-2.2328
	C	-3.29974	3.02699	-0.85321
	C	-3.3209	1.75996	0.01323
	H	-2.47342	0.6198	-1.6094
	H	-0.60834	1.66997	-0.05606
	H	0.93633	-0.30691	-0.2551
	H	-0.68666	0.09401	-2.8252
	H	-4.371	1.44056	0.05028
	H	-0.41416	-1.30581	-0.78734
	H	-0.97896	0.36732	1.05339
	H	-2.89153	-0.35219	-0.21595
	H	-3.0376	2.01556	1.04282
	H	-3.64149	2.77384	-1.86381
	H	0.95354	-0.52386	-2.69416
	H	-4.00052	3.76582	-0.44703
	N	0.74343	1.5148	-2.37373
-805.74003	N	-1.97118	3.62012	-0.98513
	H	0.08968	2.28345	-2.29738
	C	-1.47654	4.67164	-0.63829
	O	-0.889	5.65293	-0.35716
	C	2.04533	1.90331	-2.22831
	O	2.87773	0.82615	-2.15444
	O	2.41524	3.06467	-2.19619
	C	4.28257	1.13147	-2.03333
	C	4.68863	1.36343	-0.5817
	H	4.50922	2.00743	-2.64675
	H	4.78973	0.25627	-2.45103
	C	6.19715	1.60062	-0.43112
	H	4.13562	2.23012	-0.20074
	H	4.38499	0.49347	0.0168
	C	6.62006	1.83388	1.02291
	H	6.74712	0.73963	-0.83786
	H	6.49085	2.46707	-1.03976
	H	7.69956	2.00549	1.10139
	H	6.11087	2.70786	1.4464
	H	6.37287	0.96947	1.65139

Table S4. Cartesian Coordinates of the N-H-O ring precomplex

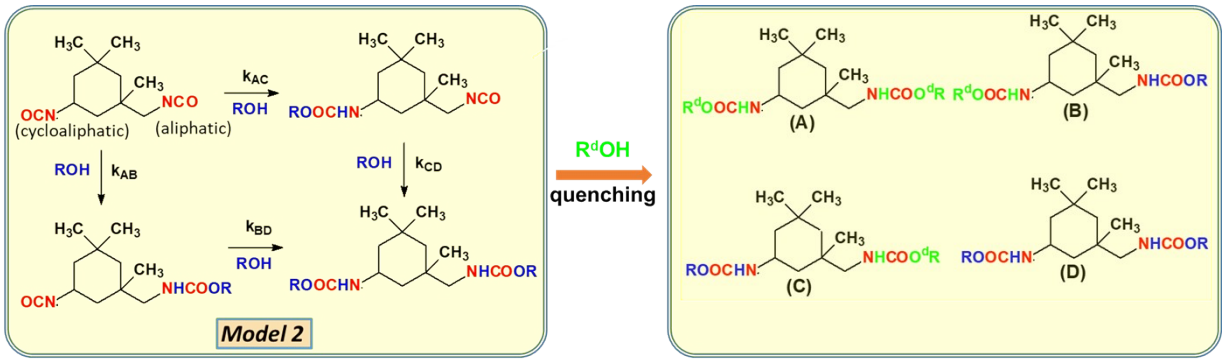
Total Energy [Hartree]	Atom	Cartesian Coordinates		
		X	Y	Z
	C	-5.65278300	1.74999800	2.00333300
	C	-7.10398900	2.04069500	1.58675300
	C	-8.12539100	1.00911200	2.09100000
	C	-8.30815500	0.95613400	3.61738900
	C	-4.71196400	4.12981000	1.76467900
	C	- 4.60410600	2.65874000	1.34122500
	H	-5.54743300	1.81978200	3.09550000
	H	-7.40860300	3.03826700	1.93068000
	H	-9.10281500	1.21866900	1.64063000
	H	-7.36632600	0.69867400	4.11286200
	H	-3.59931100	2.29903400	1.59844300
	H	-7.83225100	0.00501700	1.75251900
	H	-7.15586500	2.07017700	0.48961500
	H	-5.41172700	0.71001400	1.74393000
	H	-4.69259100	2.59767500	0.24876500
	H	-5.68446200	4.54389900	1.48515800
	H	-9.02610600	0.17130000	3.86966900
	H	-4.62772900	4.21848900	2.85596000
	N	-8.77014000	2.20794200	4.21300900
-805.74185	N	-3.70191900	4.96938000	1.15358400
	H	-8.09251200	2.86819000	4.56475100
	C	-2.52820100	4.96180900	0.88581200
	O	-1.39578100	5.09056200	0.56390100
	C	-10.04951100	2.67673000	4.23161400
	O	-10.91243700	1.77715400	3.68875800
	O	-10.37654500	3.76033600	4.69405900
	C	-12.30405600	2.16653400	3.66683800
	C	-12.63839500	3.00287700	2.43656900
	H	-12.53464400	2.71040900	4.58624400
	H	-12.85106200	1.21936000	3.66214100
	C	-14.13130100	3.35092600	2.36142500
	H	-12.04302100	3.92334600	2.46627700
	H	-12.33765700	2.44982200	1.53636600
	C	-14.48194600	4.19695200	1.13311800
	H	-14.72325100	2.42469200	2.34920300
	H	-14.42492100	3.89080200	3.27228800
	H	-15.55161800	4.43310400	1.10527400
	H	-13.92995400	5.14454400	1.13649500
	H	-14.23134800	3.67001300	0.20433700

Table S5. Cartesian Coordinates of the N-H-O ring TS

Total Energy [Hartree]	Atom	Cartesian Coordinates		
		x	y	z
	C	-2.66784460	0.70671377	0.00000000
	C	-4.08538360	1.14971877	-0.39410900
	C	-5.19849960	0.19083177	0.05757300
	C	-5.43921360	0.12850177	1.57551200
	C	-1.53516960	3.02931377	0.18479800
	C	-1.56185660	1.64263777	-0.51450800
	H	-2.58035560	0.61651477	1.09260900
	H	-4.29448160	2.15517477	-0.00327200
	H	-6.14233160	0.47899677	-0.42029100
	H	-4.52934260	-0.17610823	2.10328200
	H	-0.58678360	1.15973577	-0.38105200
	H	-4.96975460	-0.82696523	-0.28983200
	H	-4.12750560	1.24136877	-1.48788100
	H	-2.48754360	-0.30056423	-0.39975900
	H	-1.68933660	1.79167077	-1.59291200
	H	-2.34314160	3.09902077	0.91883900
	H	-6.20031660	-0.62548523	1.79185700
	H	-0.59834060	3.16547377	0.73697700
	N	-5.86990860	1.39215177	2.16944900
-805.73638	N	-1.70192360	4.14743077	-0.72214700
	H	-5.17636160	2.03311577	2.52580100
	C	1.15917660	4.66703877	-1.66255700
	O	-0.73729360	5.27523177	-2.58707500
	C	-7.13121160	1.90842477	2.15291200
	O	-8.01355660	1.03676977	1.59562800
	O	-7.42947260	3.00597177	2.60134900
	C	-9.38899760	1.47598577	1.53748400
	C	-9.66778460	2.29268177	0.28058300
	H	-9.61554860	2.05109177	2.43859200
	H	-9.97130460	0.55001177	1.54509700
	C	-11.14448760	2.69495877	0.16693600
	H	-9.03799760	3.19042777	0.29876100
	H	-9.37155660	1.70583577	-0.59947500
	C	-11.44068960	3.51578977	-1.09237800
	H	-11.77146560	1.79191977	0.17094000
	H	-11.43313760	3.27287577	1.05577300
	H	-12.49962360	3.79239577	-1.14652300
	H	-10.85185060	4.44080077	-1.10787700
	H	-11.19560460	2.95105177	-2.00017000

Table S6. Cartesian Coordinates of the N-H-O ring

Total Energy [Hartree]	Atom	Cartesian Coordinates		
		x	y	z
	C	-2.43870563	0.75188038	-0.45423976
	C	-0.97459763	1.06099038	-0.09354076
	C	0.05654637	0.31675738	-0.95702476
	C	0.24551837	0.87808838	-2.37824576
	C	-4.10497563	2.74209838	-0.34386276
	C	-3.47169463	1.54508538	0.37907024
	H	-2.61645563	0.93087038	-1.52472576
	H	-0.78542163	2.14102338	-0.14815576
	H	1.03413437	0.33528738	-0.46187776
	H	-0.71245563	0.93236738	-2.90691276
	H	-4.30657763	0.89412638	0.66782824
	H	-0.23024963	-0.74161362	-1.04112476
	H	-0.81993163	0.78735538	0.95889524
	H	-2.60481063	-0.32297862	-0.30669176
	H	-3.01404063	1.89291238	1.31349124
	H	-4.66987463	2.39852238	-1.21894876
	H	0.88803337	0.20408638	-2.95144176
	H	-4.80868963	3.24623738	0.32440624
	N	0.82625637	2.21769238	-2.41916276
-805.742	N	-3.13302463	3.73331838	-0.77262776
	H	0.19834459	3.02577628	-2.48787535
	C	-2.35834263	3.94323638	-1.66495276
	O	1.52732259	4.23973972	-2.48127565
	C	2.14493037	2.52245438	-2.28484976
	O	2.90377137	1.39579638	-2.16297176
	O	2.59762437	3.65855638	-2.28718176
	C	4.32475437	1.60206238	-2.01674076
	C	4.71656637	1.82650038	-0.56015876
	H	4.62774237	2.44789138	2.44789138
	H	4.77609837	0.68628838	0.68628838
	C	6.23493237	1.95745438	1.95745438
	H	4.21905737	2.73540238	2.73540238
	H	4.34003537	0.98921038	0.98921038
	C	6.64410637	2.17781438	2.17781438
	H	6.72859837	1.05381338	1.05381338
	H	6.60234537	2.79261238	2.79261238
	H	7.73158637	2.27061738	2.27061738
	H	6.19232837	3.09229438	3.09229438
	H	6.32110637	1.34175938	1.34175938



Scheme S1. Reaction pathways for IPDI

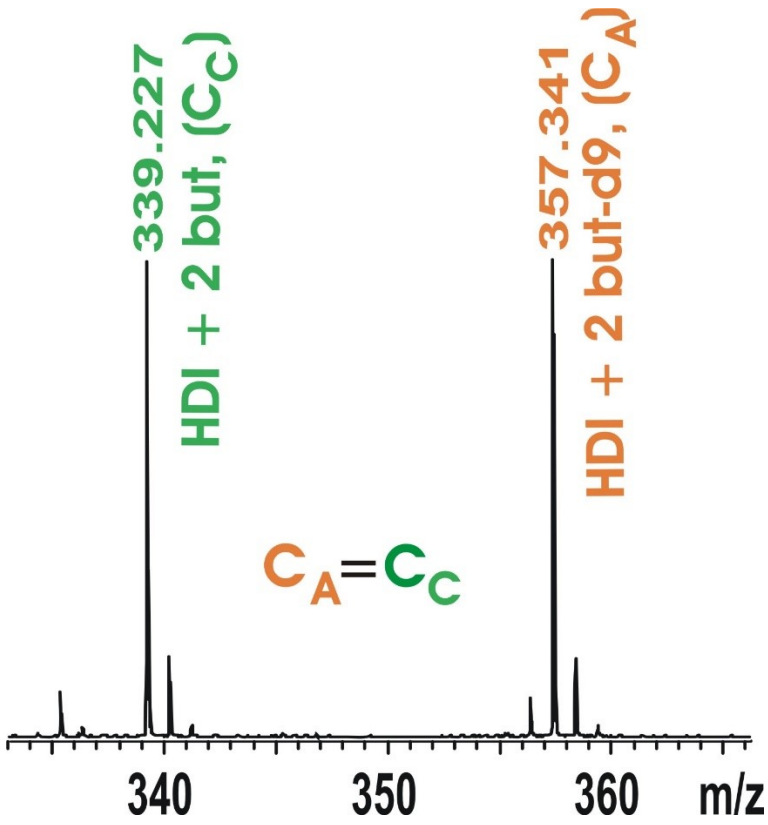


Figure S1. The zoomed ESI-MS spectrum obtained from the equimolar mixture of HDI adduct with 2 molecules butan-1-ol (C) and HDI adduct with 2 molecules d9-butan-1-ol (A).