Supplementary Materials

New Polymers In Silico Generation and Properties Prediction

Andrey A. Knizhnik [1,2], Pavel V. Komarov [3,4,*], Boris V. Potapkin [1,2], Denis B. Shirabaykin [1], Alexander S. Sinitsa [1,2] and Sergey V. Trepalin [1,5]

[1] Kintech Lab Ltd., 3rd Khoroshevskaya Str. 12, Moscow, 123298 Moscow, Russia
[2] National Research Center "Kurchatov Institute", Akademika Kurchatova Sq., 1, 123182 Moscow, Russia
[3] Institute of Organoelement Compounds RAS, Vavilova St. 28, 119991 Moscow, Russia
[4] General Physics Department, Tver State University, Sadovy Str. 35, 170002 Tver, Russia
[5] All Russian Institute for Scientific and Technical Information RAS, Usievicha Str. 20, 125215 Moscow, Russia
* Correspondence: pv_komarov@mail.ru

Additional Figures and Tables mentioned in the main text of our article.

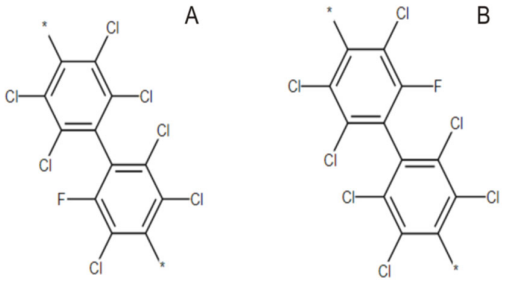


Figure S1. Identical structures for which different InChIkeys are generated (we tested the "winchi-1.exe" program included in the InChI 1.06 [48] distribution kit). The structure (A) InChIKey = BOJVIOJYDPQJAU-GDRMAEQFBA-N differs from structure (B) InChIKey = BOJVIOJYDPQJAU-SZAYNCSKBA-N by a 180-degree rotation in the plane.

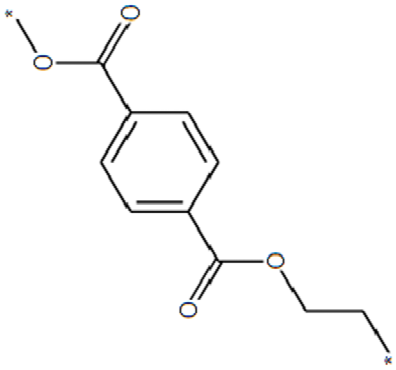


Figure S2. An example of the output of property prediction results for polyethylene terephthalate is shown in Table S1.

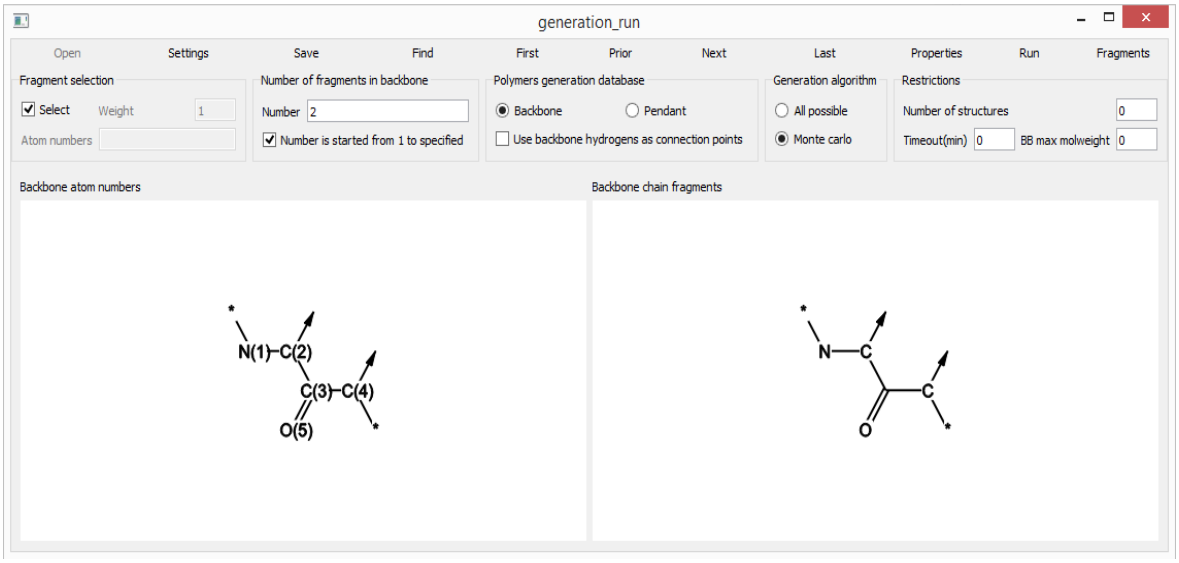


Figure S3. The graphical interface for setting initial conditions for the generation of structures. The isotopic labels of the compound in the database are interpreted as connecting points of pendant groups (arrows in the figure) and as flags of the backbone continuation (atoms to which asterisks are attached).

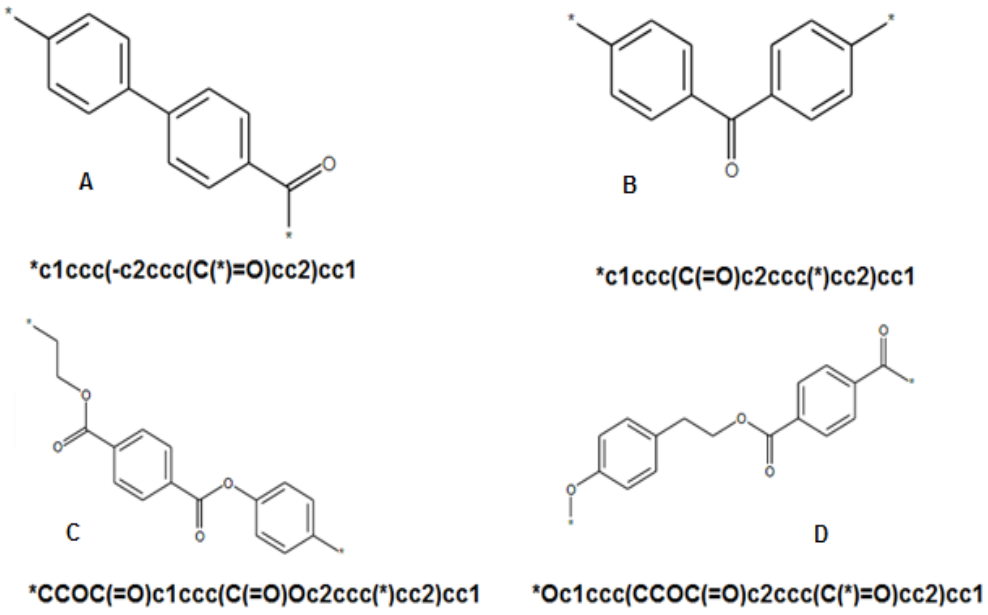


Figure S4. Example of duplicates in the PI1M database with the given SMILES notation. The pairs of structures (A, B) and (C, D) are identical. They differ in the choice of SRU, which is not unique.

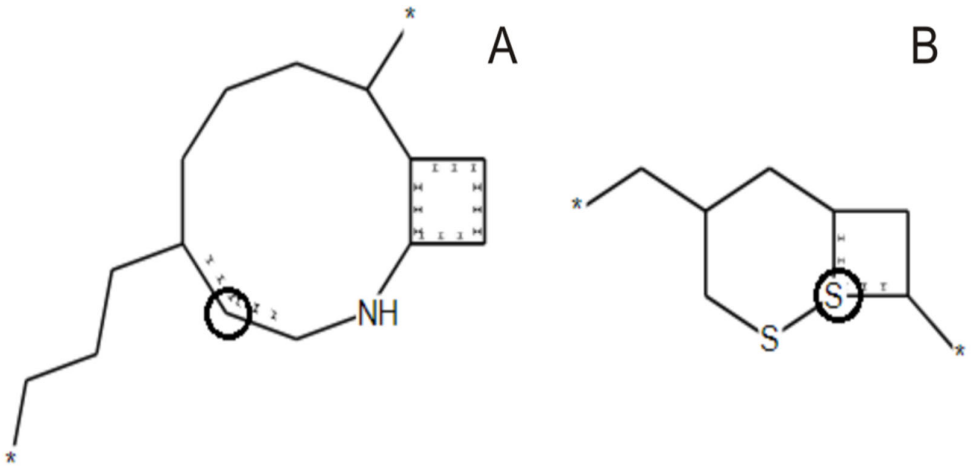
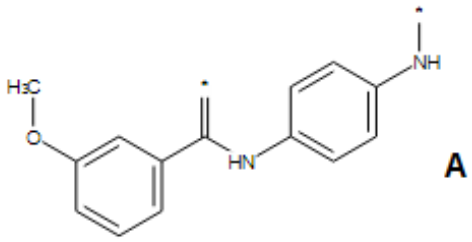


Figure S5. Examples of compounds (taken from PI1M) with aromatic cycles that do not clearly alternating for single and double bonds. One of the aromatic bonds on the circled atoms: (A) carbone, (B) sulfur must be single, and the other must be double. Because of the uncertainty, it is not possible to count the number of hydrogen atoms in neighboring atoms.



Nc1ccc(NC(=)c2cccc(OC)c2)cc1

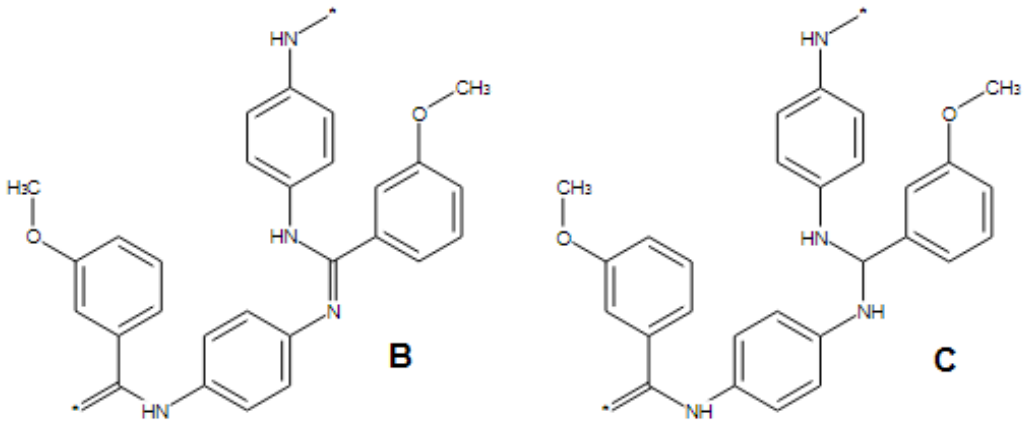


Figure S6. A repeating polymer fragment (A) and two possible dimers (B and C) that can be generated from fragment A. The dimers differ by the presence (B) and absence (C) of the double bond C=N/C-N.

Table S1. Results of the prediction of the properties of polyethylene terephthalate (see Figure S1).

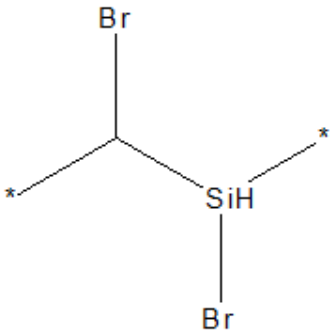
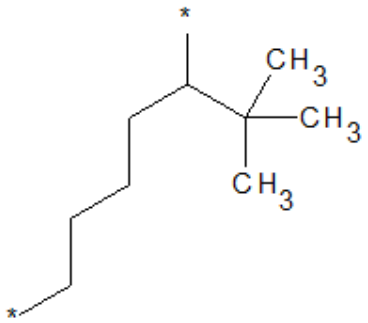
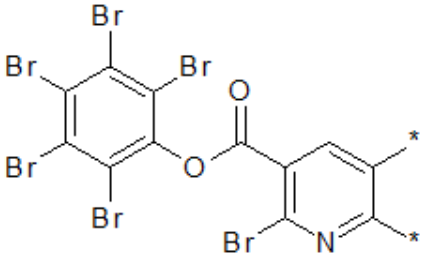
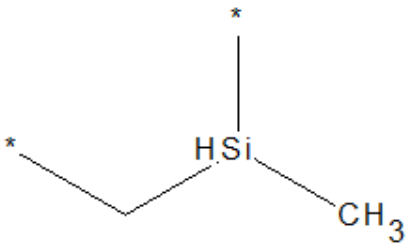
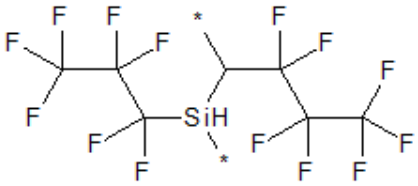
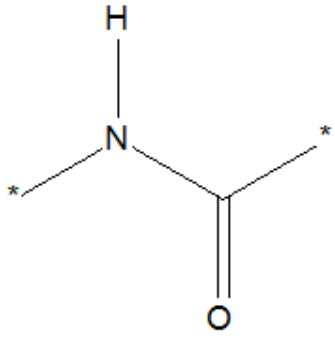
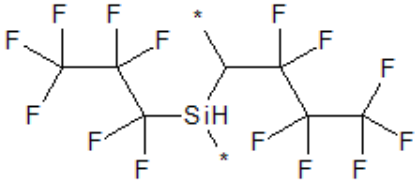
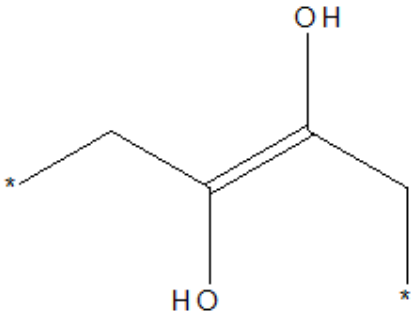
Property name	Abbreviation	Value	Units of measure
Connectivity index 0X	$^0\chi$	9.966255	
Connectivity index 0Xv	$^0\chi^v$	7.356608	
Connectivity index 1X	$^1\chi$	6.770857	
Connectivity index 1Xv	$^1\chi^v$	4.215214	
Repeat unit number of atoms	NAtoms	22	
Repeat unit number of non-hydrogen atoms	NNonH	14	
Molweight PRU	mw	192.171120	g/mole
Van-der-Waals Volume	V_w	95.043400	cm^3/mole
Molar Volume	V	145.906844	cm^3/mole
Polymer Molweight	mw	100000.000000	g/mole
Density	d	1.317081	g/cm^3
HeatCapacity(liquid)	$C_{(l)}$	311.476898	J/mole/K
HeatCapacity(solid)	$C_{(s)}$	228.868423	J/mole/K
Cohesion Energy Fedors	ECoh1	74086.000000	J/mole
Cohesion Energy Van Krevelen	ECoh2	57031.144728	J/mole
Solubility parameter Feudor	δ	22.533582	$(J/cc)^{0.5}$
Solubility parameter VanKrevelen	δ	19.770525	$(J/cc)^{0.5}$
Refractive Index	n_D	1.555804	
Molar Refractivity	R_{LL}	46.886865	cm^3/mole
Dielectric constant	ε	3.282741	
Molar Polarizability	P_{LL}	63.048247	cm^3/mole
Effective dipole Moment	μ	0.885737	Debye
Glass temperature at molweight 100000.000000	T_g	369.530916	K
Infinite molweight Tg	$T_g$inf	368.160911	K
Bulk modulus	B	4411.275179	MPa
Young modulus	E	2594.893883	MPa
Shear modulus	G	925.452316	MPa
Entanglement Molweight	me	5732.790343	g/mole
Brittle fracture stress at infinite molweight	$\sigma_f(\infty)$	112.761375	Mpa
Brittle fracture stress at molweight 100000.000000	$\sigma_f(\infty)$	90.782506	Mpa
Yield stress	σ_y	72.657029	Mpa
PRU length (used)	l	7.189514	A
Molar Rao function	U_R	8568.091706	$cm^{10/3}/(sec^{1/3}mole)$
Molar Hartman function	U_H	6596.460723	$cm^{10/3}/(sec^{1/3}mole)$
Poisson ratio	nu	0.401960	
Molar stiffness function	K	80.936657	$g^{0.25}cm^{1.5}/mole^{0.75}$
Molar viscosity function	H_η	7001.243871	$g*J^{1/3}*mole^{-4/3}$
Activation energy viscous flow	E_η	48.357212	kJ/mol
Thermal conductivity at 298K	$\lambda(298)$	0.209668	J/(K*m*sec)
Permeability of oxygen at 298K	P_{O2}	0.039764	Barrers

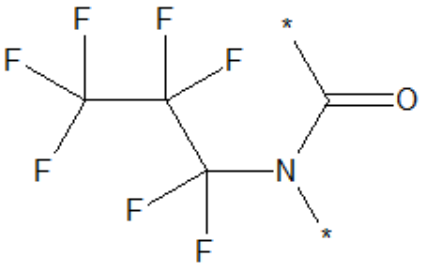
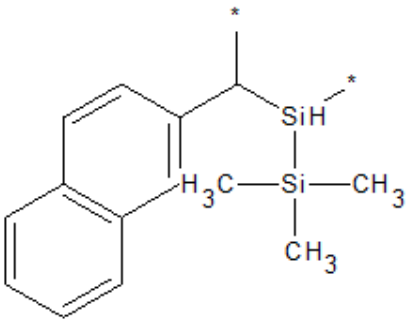
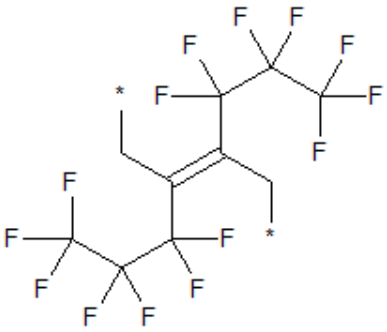
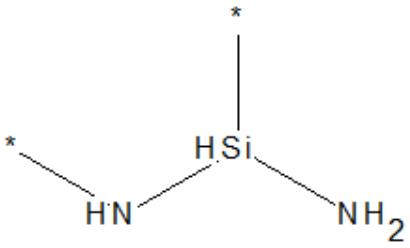
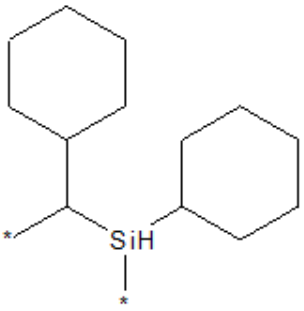
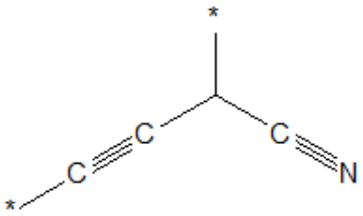
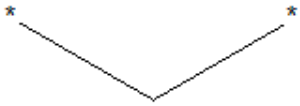
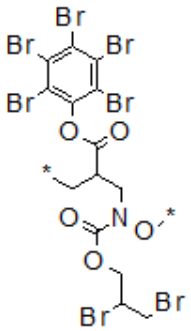
Property name	Abbreviation	Value	Units of measure
Permeability of nitrogen at 298K	P_{N2}	0.007916	Barrers
Permeability of carbon dioxide at 298K	P_{CO2}	0.137064	Barrers
Permeability of water vapours at 298K	P_{H2O}	87.849412	Barrers
Molar Thermal Decomposition function	$Y_{d,1/2}$	140.650619	K*kg/mol
Temperature of half decomposition	$T_{d,1/2}$	731.903000	K
Soluble in solvents		Morpholine, Pyridine, Cellosolve	
Insoluble in solvents		Ethylene glycol, Glycerol, Water	

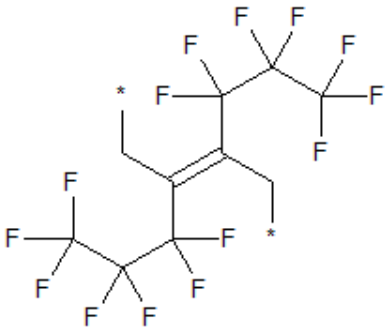
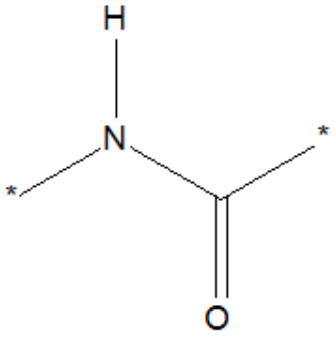
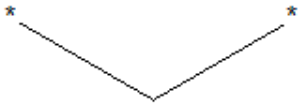
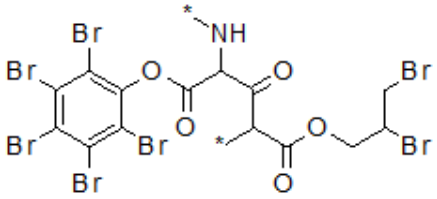
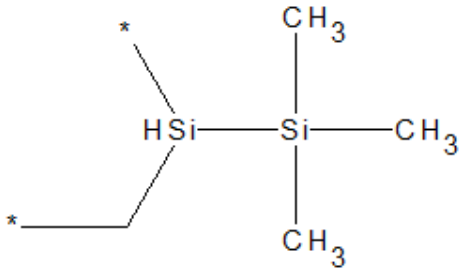
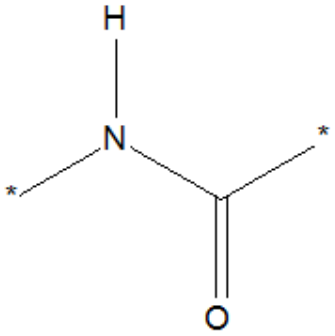
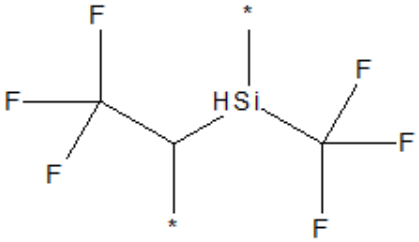
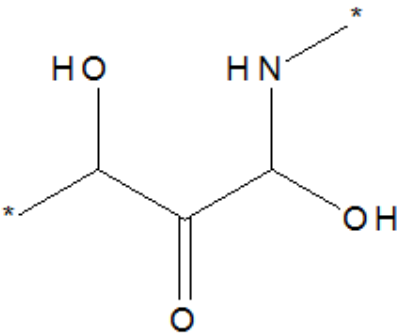
Table S2. Extreme values of the predicted physicochemical properties of polymers with various combinations of substituents and BiceranoDB polymers [11]. The explanation of property abbreviations is given in Table S1. MinID and MaxID are identifiers of structures in the ZeroTwo.zip database [53]. For properties, dependent on molecular weight, the molecular weight of the polymer was assumed to be 100,000.

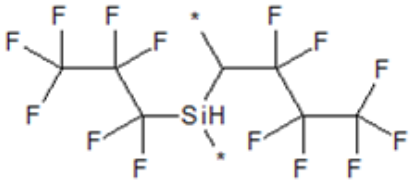
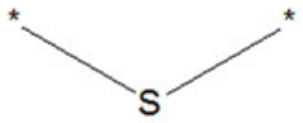
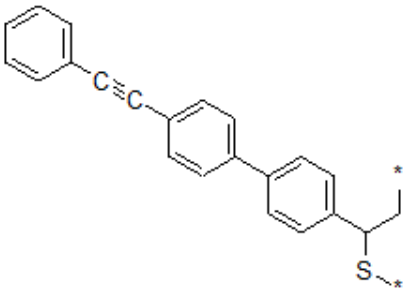
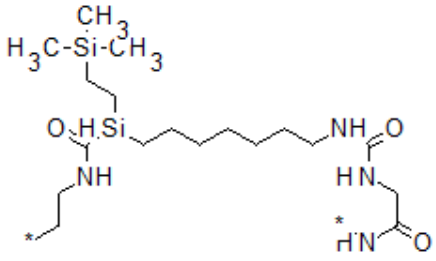
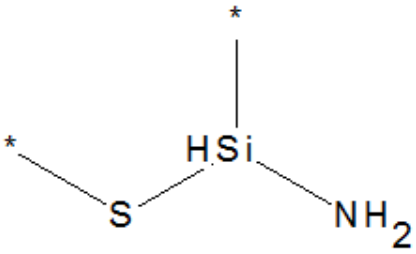
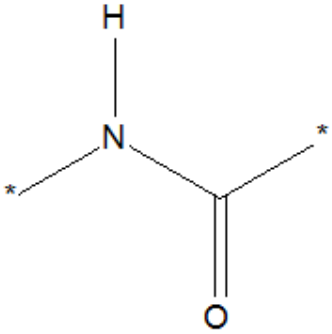
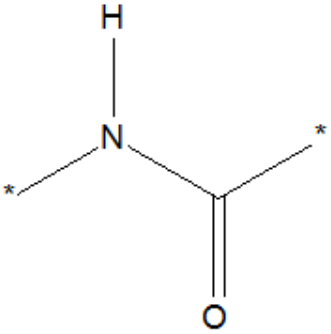
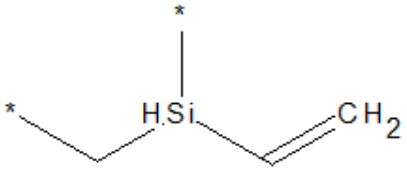
	ZeroTwo structures (5,142,153)				Bicerano DB(811)	
Property	**Min.**	**Min.ID**	**Max.**	**Max. ID**	**Min.**	**Max.**
CL	0.7959	A2706088	2.222	A1571904	0.8735	2.286
CS	0.5638	A1193001	1.859	A2695849	0.5344	1.805
COH1	161	A2774968	1321	A3195731	160.9	1321
COH2	85.06	A2774968	1016	A0722505	74.92	982.9
RLL	0.1108	A3195737	0.3527	A2773598	0.1008	0.3598
PLL	0.1506	A0719754	0.5080	A0614124	0.1189	0.4673
EAFLOW	0.04.998	A2786776	3.666	A1514456	0.03678	5.486
STIFFNESS	6.410	A2914202	228.4	A1590739	10.38	383.7
EPSILON	2.126	A0719754	9.404	A3195731	2.004	9.404
VISCFUNC	392.7	A2914202	37440	A0023354	785.4	37260
DELTA1	13.30	A2695772	47.21	A3195731	13.76	47.21
DELTA2	12.33	A2789072	38.23	A0054943	12.55	34.81
N	1.338	A2774968	1.828	A1979974	1.332	1.828
MU	0.000	A0283413	1.876	A0000575	0.000	1.990
MB	379.9	A2257247	23550	A3195731	529.3	23550
O2PERM	1.16×10^{-14}	A3195731	129.7	A2695845	1.16×10^{-14}	82.19
N2PERM	2.27×10^{-16}	A3195731	49.45	A2695845	2.28×10^{-16}	30.22
CO2PERM	3.05×10^{-15}	A3195731	920.1	A2695845	3.05×10^{-15}	560
TDECOMP	451.8	A1210993	1162	A2257316	484.5	1098
SINF	10.19	A2797603	652.3	A3027335	7.625	317.8
SIGMAF	1.57×10^{-5}	A0866414	629	A3027335	0.6623	301.6
SIGMAY	3.179	A2257344	337.3	A1194543	13.20	302.9

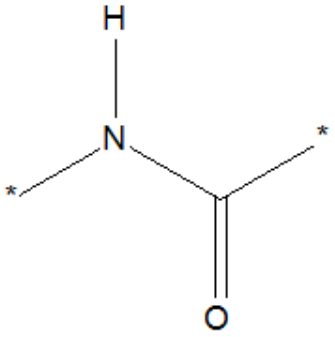
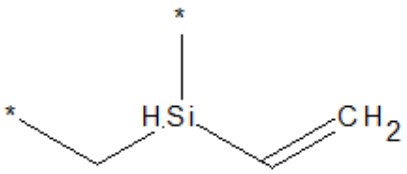
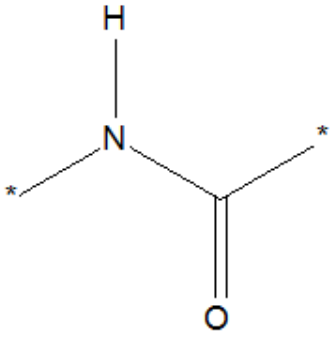
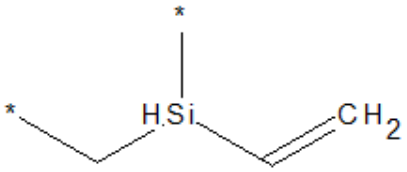
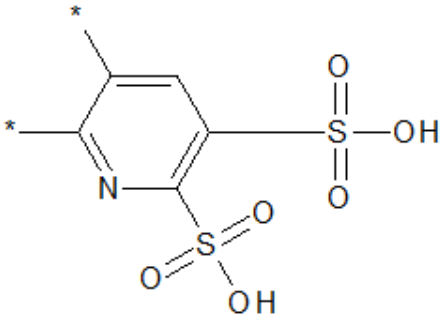
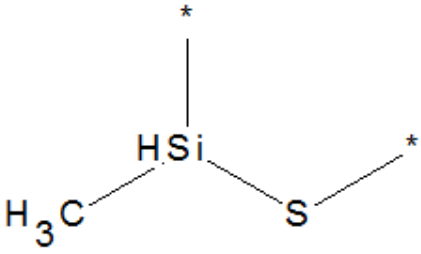
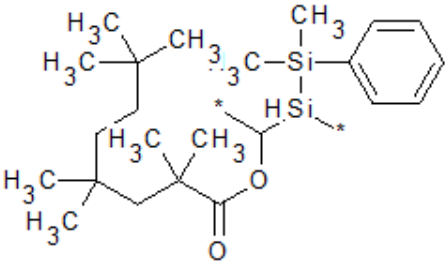
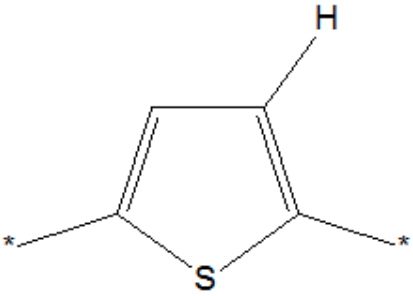
Table S3. Chemical structures with extreme property values in the ZeroTwo database [53].

Property name	Minimal value	Maximal value
CL J/g/K	 0.7959	 2.222
CS J/g/K	 0.5638	 1.859
COH1 J/g	 161	 1.321E+3
COH2 J/g	 85.06	 1.016E+3

Property name	Minimal value	Maximal value
RLL cm^3/g		
	0.1108	0.3527
PLL cm^3/g		
	0.1506	0.5080
EAFLOW kJ/g		
	4.998E-2	3.666
STIFFNESS $g^{0.25}cm^{1.5}/mole^{0.75}$		
	6.410	228.4

Property name	Minimal value	Maximal value
EPSILON		
	2.126	9.404
VISCFUNC g*J$^{1/3}$*mole$^{-4/3}$		
	392.7	3.744E+4
DELTA1 (J/cc)$^{0.5}$		
	13.30	47.21
DELTA2 (J/cc)$^{0.5}$		
	12.33	38.23

Property name	Minimal value	Maximal value
N		
MU Debye	 0.000	 1.876
MB MPa	 379.9	 2.355E+4
O2PERM Barrers	 1.163E-14	 129.7

Property name	Minimal value	Maximal value
N2PERM Barrers		
	2.278E-16	49.45
CO2PERM Barrers		
	3.050E-15	920.1
TDECOMPK		
	451.8	1.162E+3
SINF MPa		
	10.19	652.3

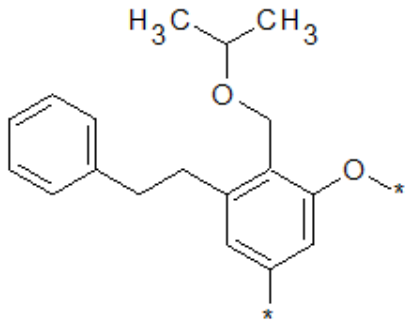
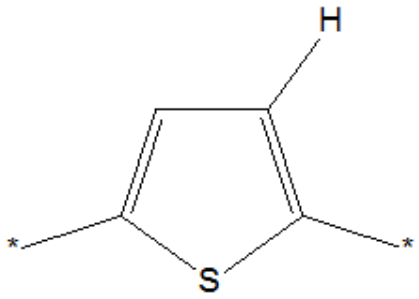
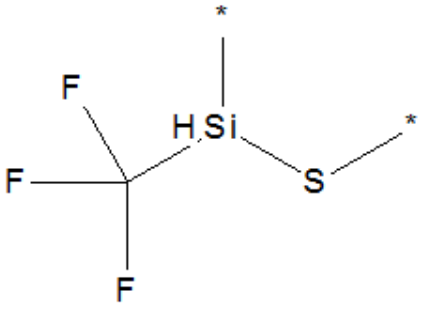
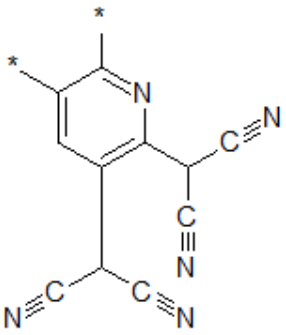
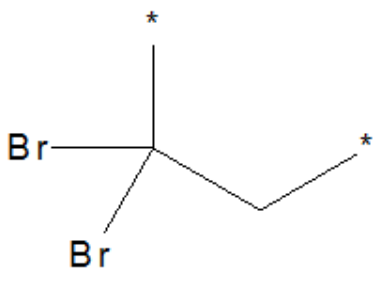
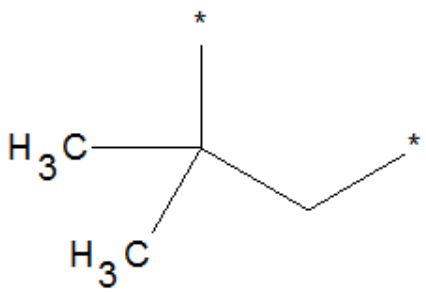
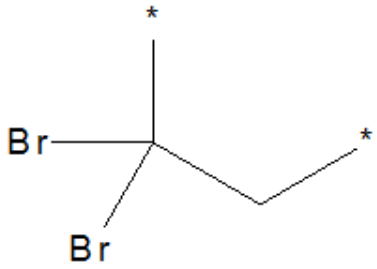
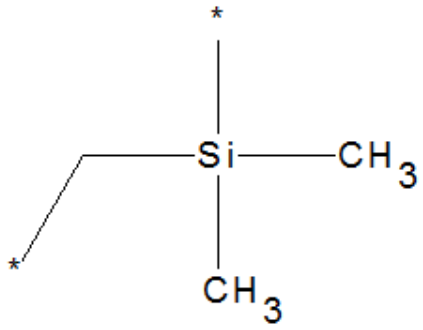
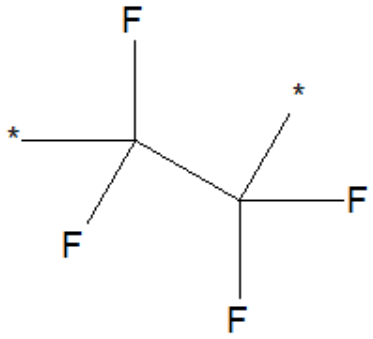
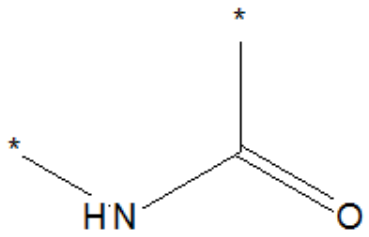
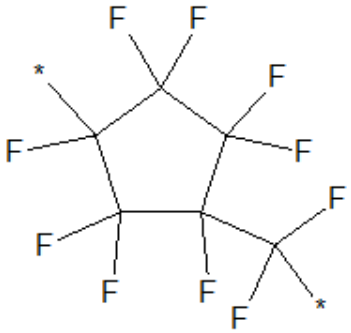
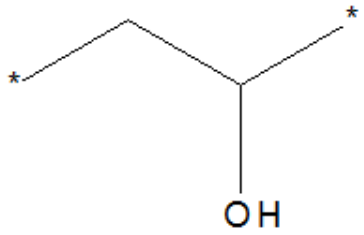
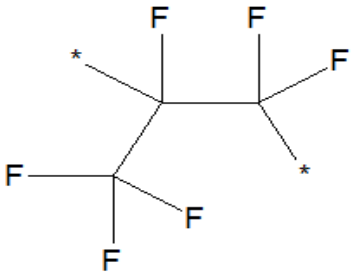
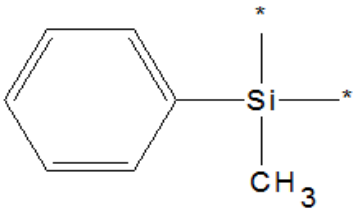
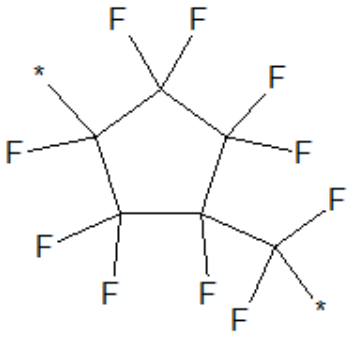
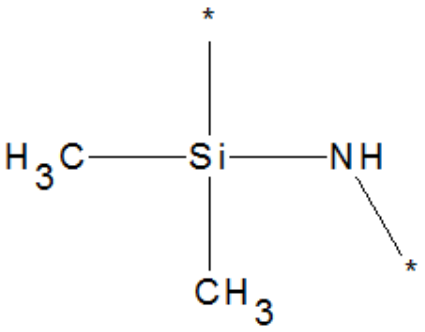
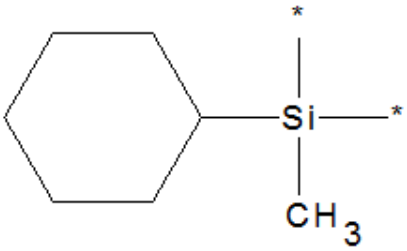
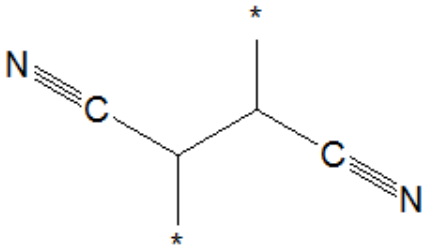
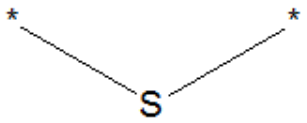
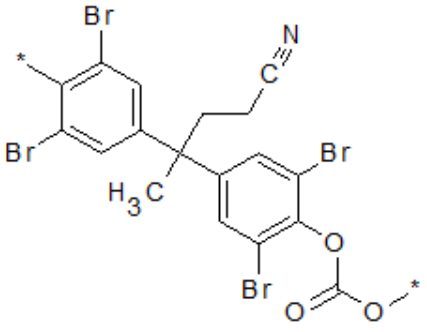
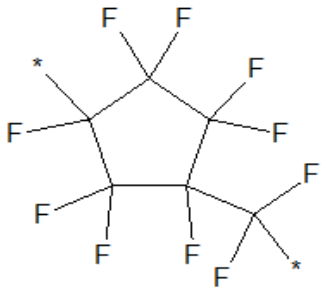
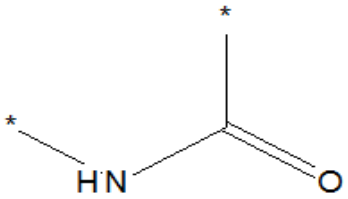
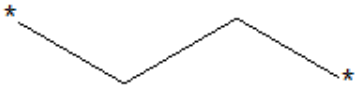
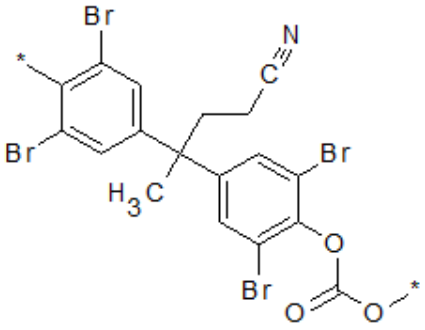
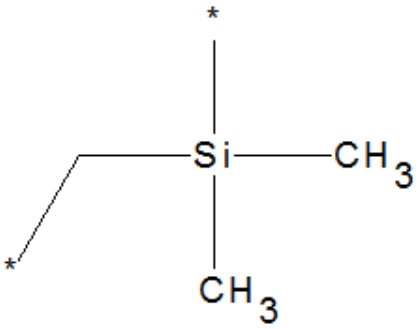
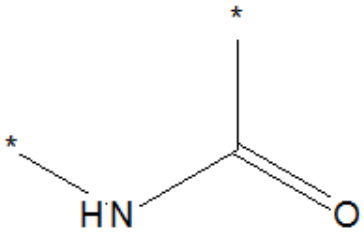
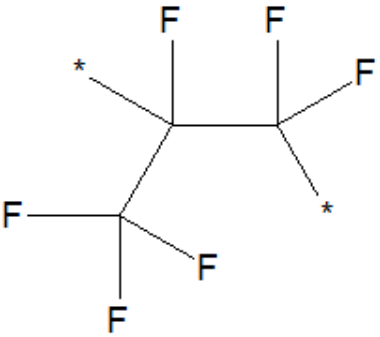
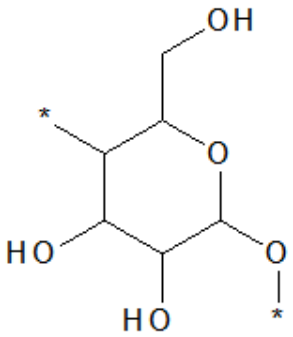
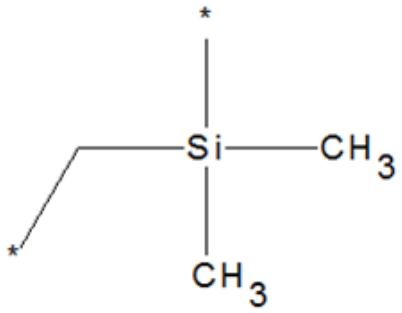
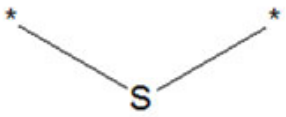
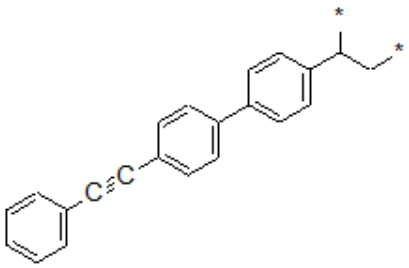
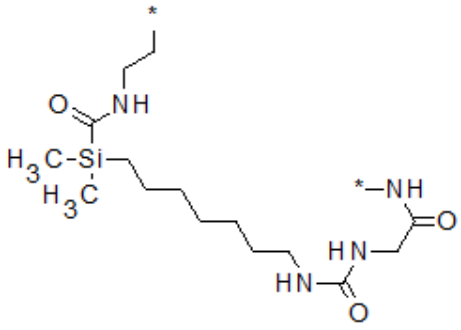
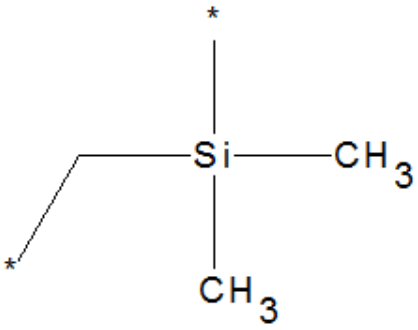
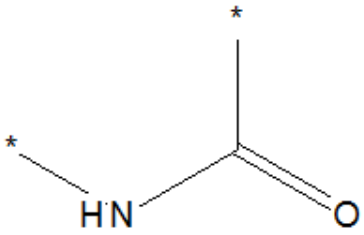
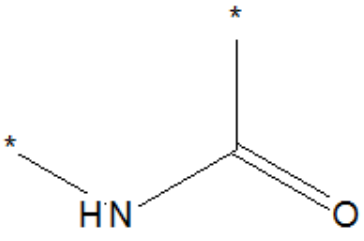
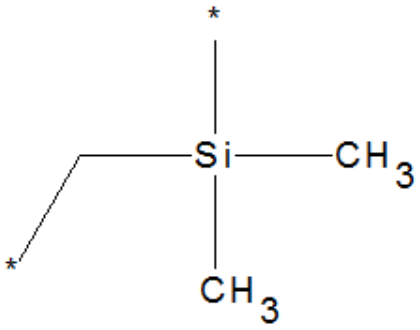
Property name	Minimal value	Maximal value
SIGMAF MPa		
	1.573E-5	629
SIGMAY MPa		
	3.179	337.3

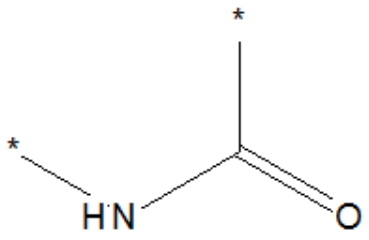
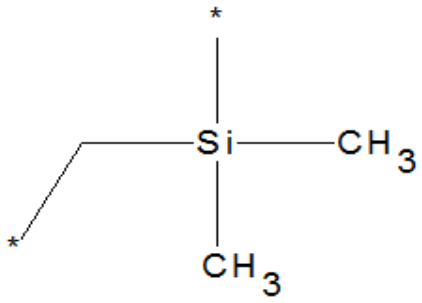
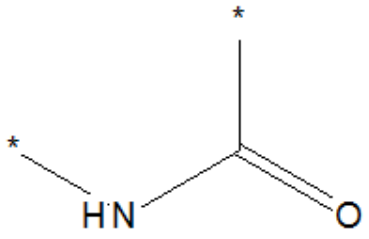
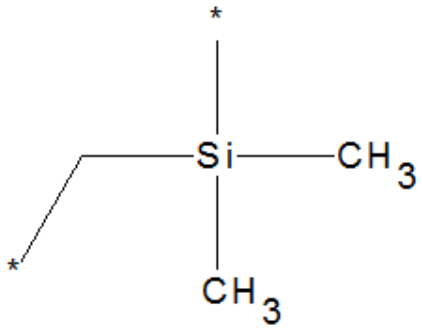
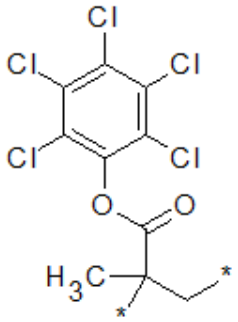
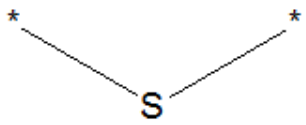
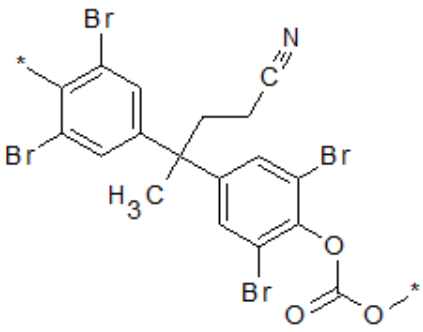
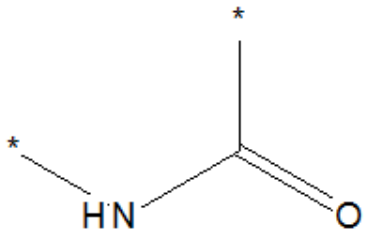
Table S4 . Chemical structures with extreme values of properties in the Bicerano database [11].

Property name	Minimal value	Maximal value
CL J/g/K		
	0.8735	2.286
CS J/g/K		
	0.5344	1.805
COH1 J/g		
	160.9	1.321E+3
COH2 J/g		
	74.92	982.9

Property name	Minimal value	Maximal value
RLL cm^3/g		
	0.1008	0.3598
PLL cm^3/g		
	0.1189	0.4673
EAFLOW kJ/g		
	7.252E-2	5.486
STIFFNESS $g^{0.25}cm^{1.5}/mole^{0.75}$		
	10.38	223.7

Property name	Minimal value	Maximal value
EPSILON		
	2.004	9.404
VISCFUNC g*J$^{1/3}$*mole$^{-4/3}$		
	785.4	2.964E+4
DELTA1 (J/cc)$^{0.5}$		
	13.76	47.21
DELTA2 (J/cc)$^{0.5}$		
	12.55	34.81

Property name	Minimal value	Maximal value
N		
MU Debye		
	0.000	1.733
MB MPa		
	529.3	2.355E+4
O2PERM Barrers		
	1.163E-14	82.19

Property name	Minimal value	Maximal value
N2PERM Barrers	 2.278E-16	 30.22
CO2PERM Barrers	 3.050E-15	 560
TDECOMP K	 484.5	 1.098E+3
SINF MPa	 13.69	 317.8

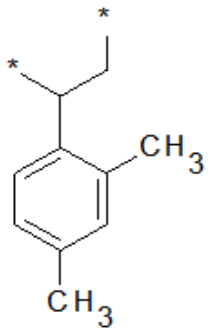
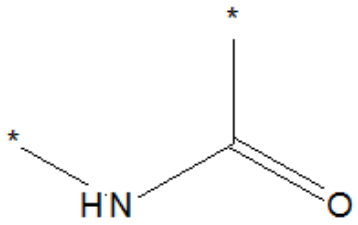
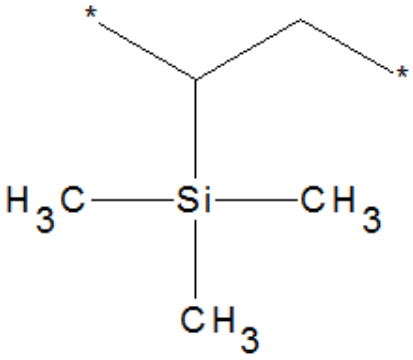
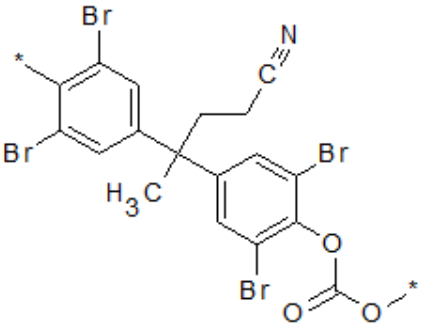
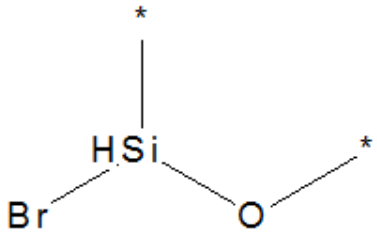
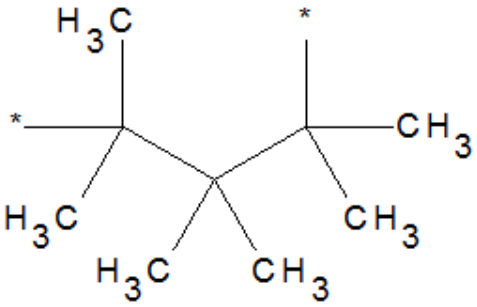
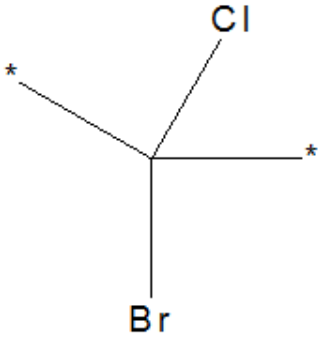
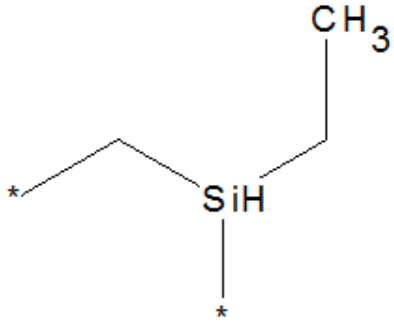
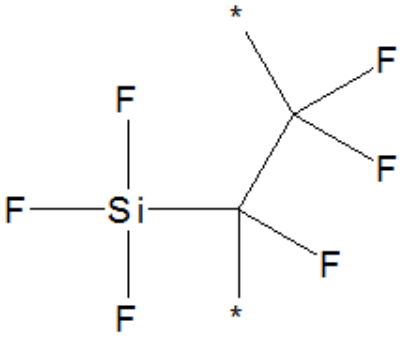
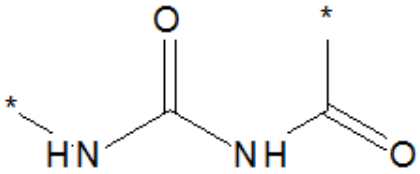
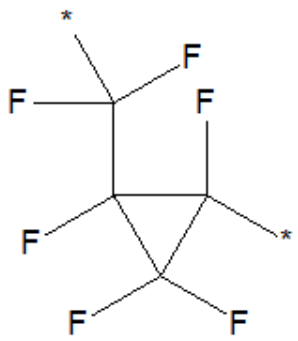
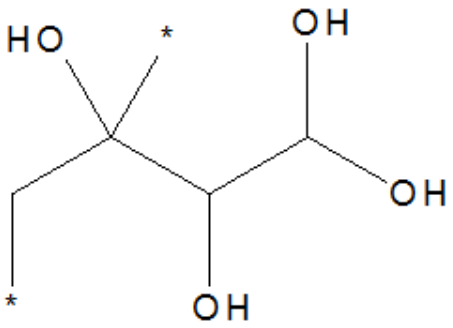
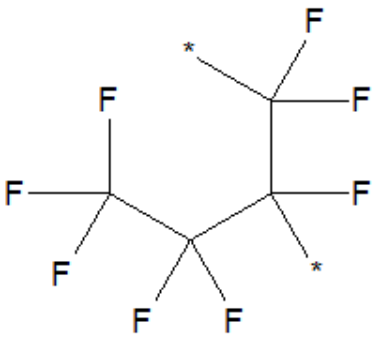
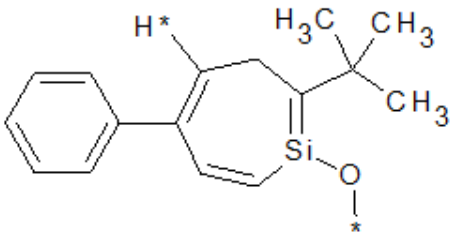
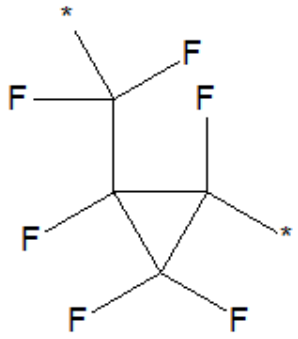
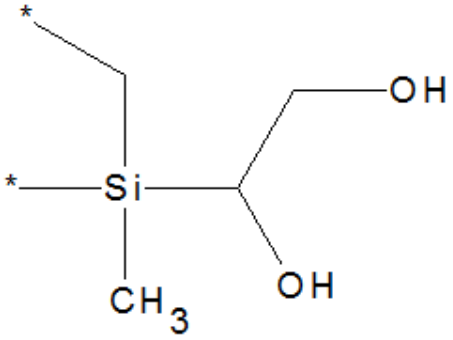
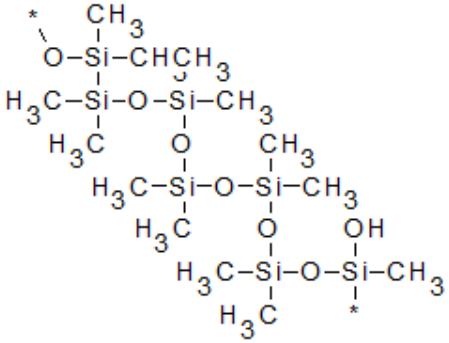
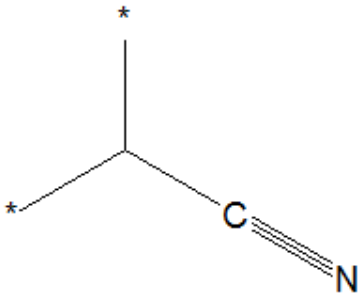
Property name	Minimal value	Maximal value
SIGMAF MPa	 0.6623	 301.6
SIGMAY MPa	 13.20	 283.2

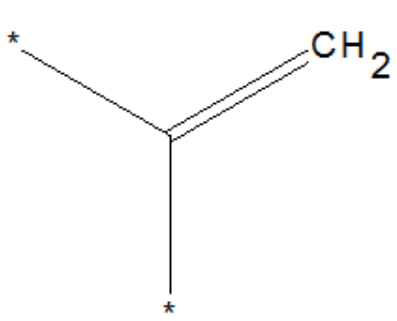
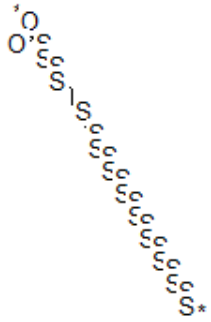
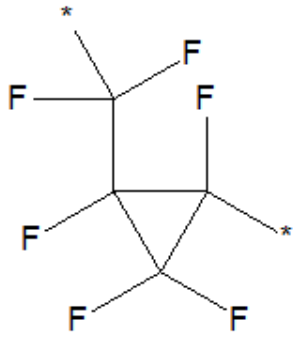
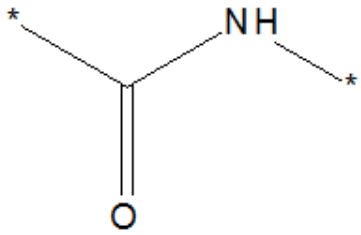
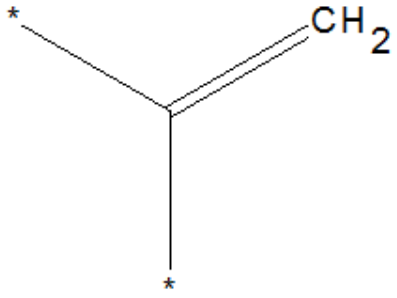
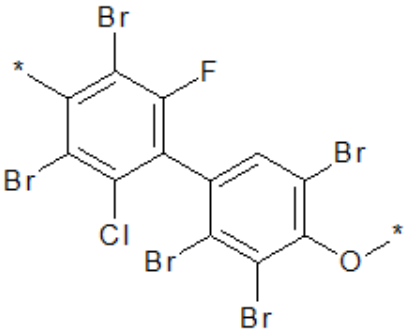
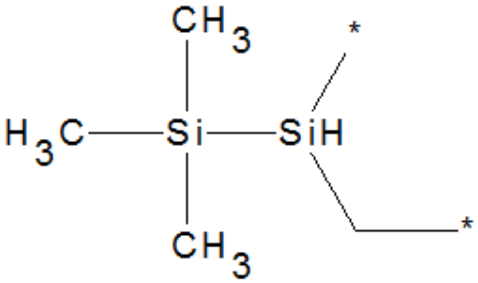
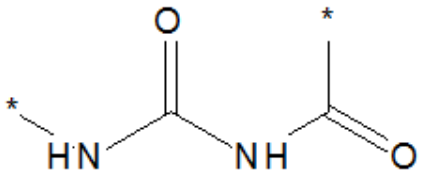
Table S5 Extreme values of the predicted properties of compounds from the PI1M database [54] and the Monte Carlo database [53] (see our open-access file MonteCarloSmi.zip). For molecular weight-dependent properties, the molecular weight of the polymer was assumed to be 100,000. The abbreviated property names are listed in Table 1. Min.ID and Max.ID are identifiers of structures in the MonteCarloSmi.zip database [53].

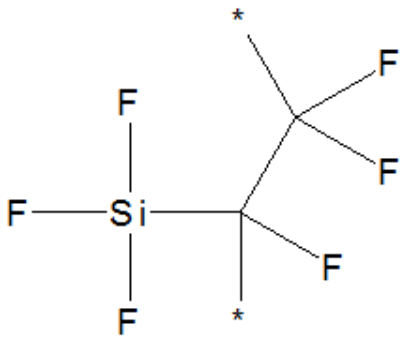
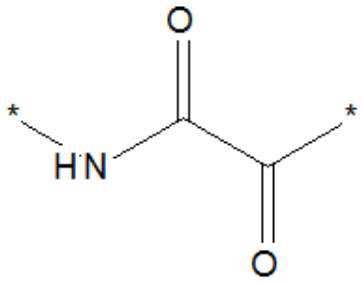
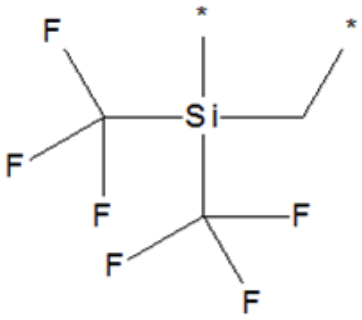
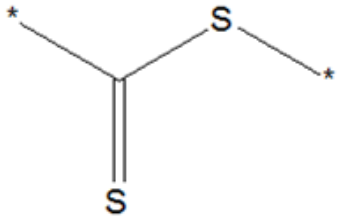
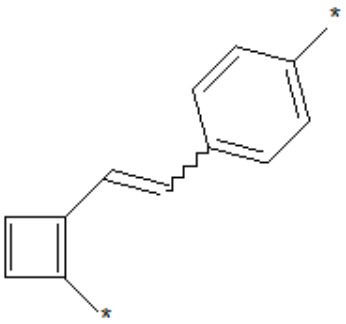
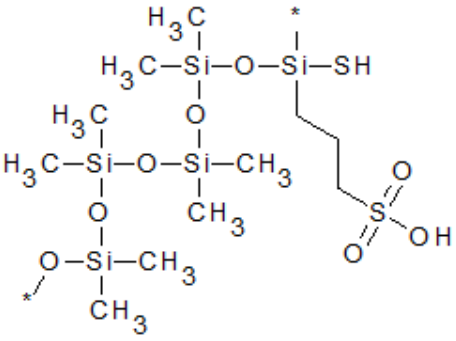
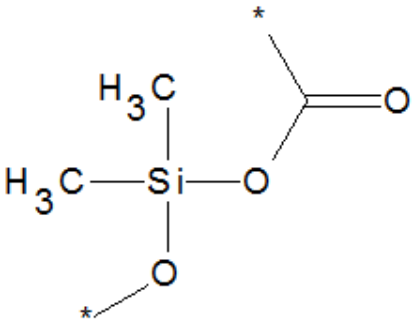
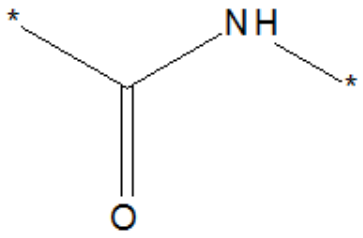
PI1M (787740 records)			**Monte Carlo (787740)**			
Property name	**Min.**	**Max.**	**Min**	**Min.ID**	**Max**	**MaxID**
CL	0.8326	2.320	0.7372	M462816	2.257	M001119
CS	0.5292	1.912	0.5450	M176330	1.956	M378740
COH1	121.8	1321	142.4	M386809	1321	M158906
COH2	73.42	1287	84.18	M085666	1296	M417124
RLL	0.1008	0.4047	0.1074	M028780	0.4158	M321639
PLL	0.1122	0.4923	0.1379	M028780	0.5319	M081557
EAFLOW	0.01369	10.97	0.01655	M620408	10.97	M296756
STIFFNESS	4.725	650.8	6.719	M097818	977.4	M726398
EPSILON	1.950	9.404	2.110	M028780	9.404	M001322
VISCFUNC	750.8	50200	781.6	M102345	177600	M726398
DELTA1	12.60	47.21	12.60	M378740	47.21	M158906
DELTA2	10.07	44.12	11.54	M117435	44.12	M001722
N	1.320	1.889	1.341	M028780	1.826	M316810
MU	0.000	2.999	0.000	M000046	4.086	M503372
MB	277.6	23550	207.3	M170848	23550	M001322
O2PERM	5.798×10^{-15}	458.7	5.798×10^{-15}	M158906	461.2	M075166
N2PERM	1.074×10^{-16}	193.6	1.074×10^{-16}	M158906	194.8	M075166
CO2PERM	1.429×10^{-15}	3644	1.429×10^{-15}	M158906	3666	M075166
TDECOMP	363.7	1266	368.9	M125581	1319	M378740
SINF	2.664	894.4	0.8548	M598491	2424	M000121
SIGMAF	4.055×10^{-5}	862.2	4.365×10^{-3}	M014023	2339	M000121
SIGMAY	4.064	719.5	0.2152	M075166	758.8	M598491

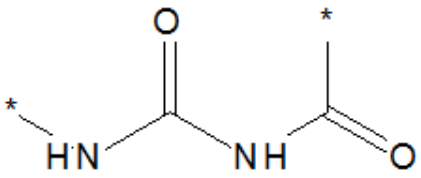
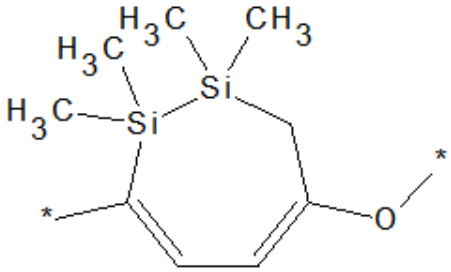
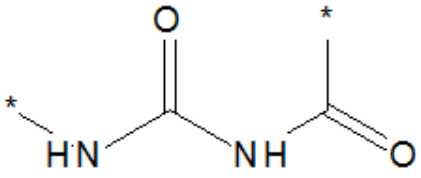
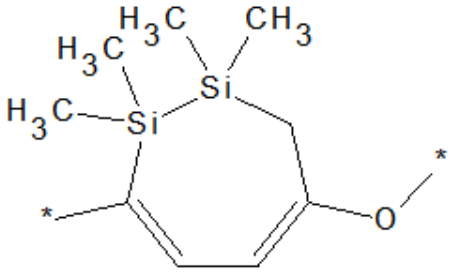
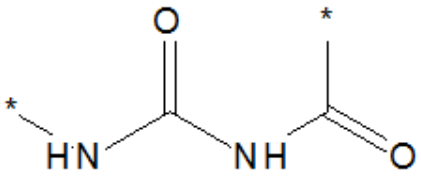
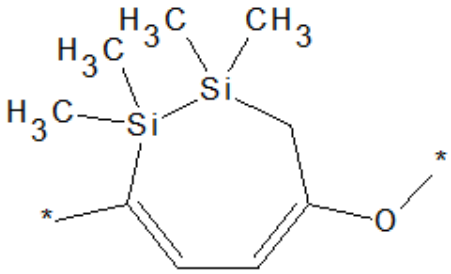
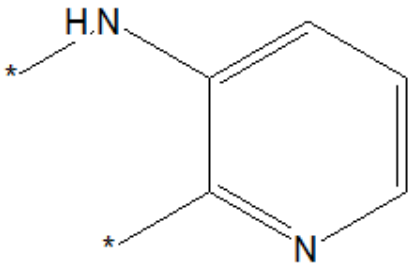
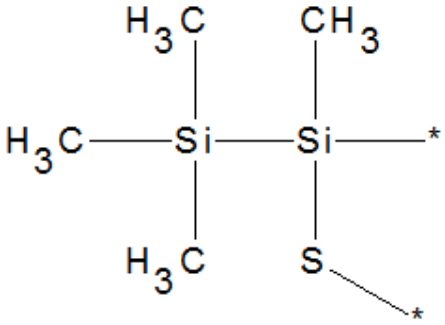
Table S6. Chemical structures with extreme property values from the PI1M database [35].

Property name	Minimal value	Maximal value
CL J/g/K		
	0.8326	2.320
CS J/g/K		
	0.5292	1.843
COH1 J/g		
	145.4	1.321E+3

Property name	Minimal value	Maximal value
COH2 J/g	 73.84	 1.287E+3
RLL cm^3/g	 0.1008	 0.3881
PLL cm^3/g	 0.1122	 0.4857
EAFLOW kJ/g	 2.851E-2	 10.97

Property name	Minimal value	Maximal value
STIFFNESS $g^{0.25}cm^{1.5}/mole^{0.75}$		
	4.725	254.6
EPSILON		
	1.950	9.404
VISCFUNC $g*J^{1/3}*mole^{-4/3}$		
	750.8	2.891E+4
DELTA1 $(J/cc)^{0.5}$		
	13.30	47.21

Property name	Minimal value	Maximal value
DELTA2 $(J/cc)^{0.5}$		
	11.39	44.12
N		
MU Debye		
	0.000	1.997
MB MPa		
	277.6	2.355E+4

Property name	Minimal value	Maximal value
O2PERM Barrers		
	5.798E-15	347.4
N2PERM Barrers		
	1.074E-16	143.4
CO2PERM Barrers		
	1.429E-15	2.692E+3
TDECOMPK		
	363.7	1.116E+3

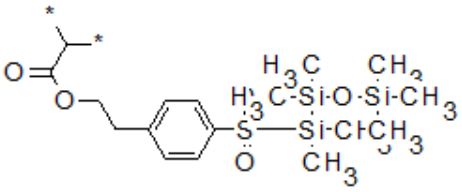
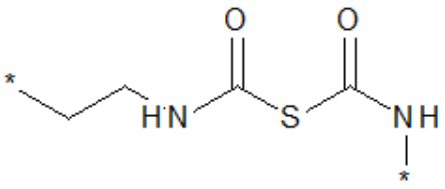
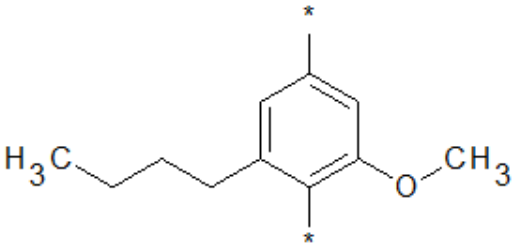
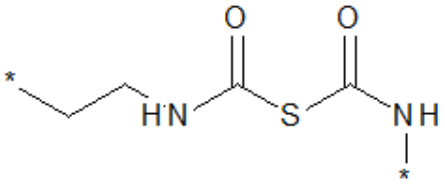
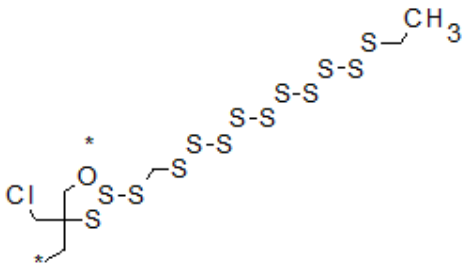
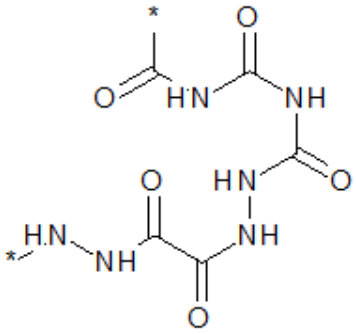
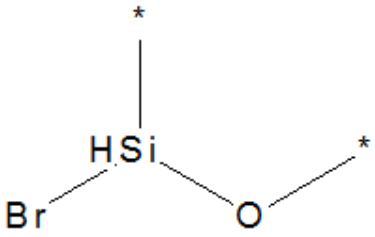
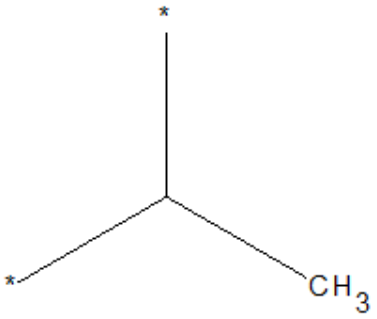
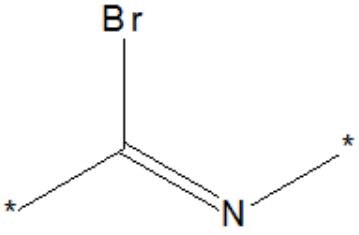
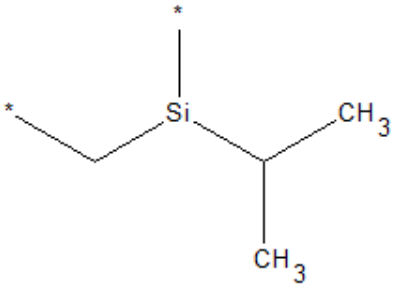
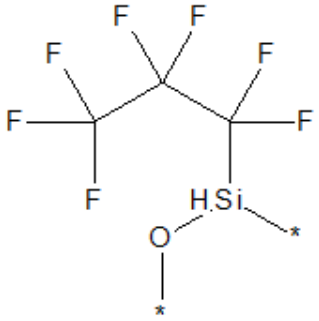
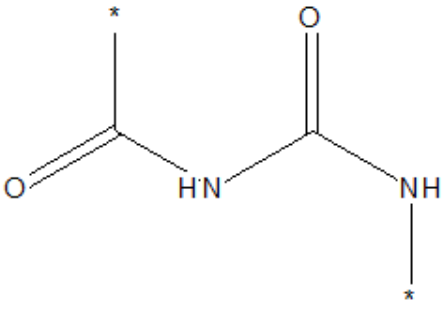
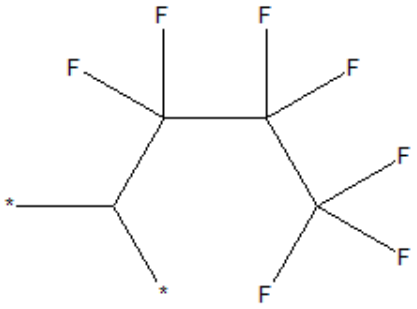
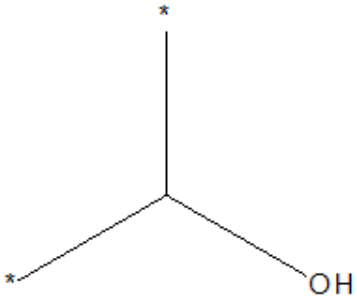
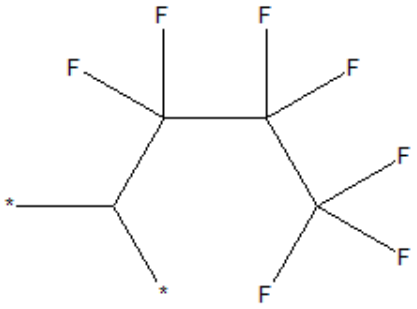
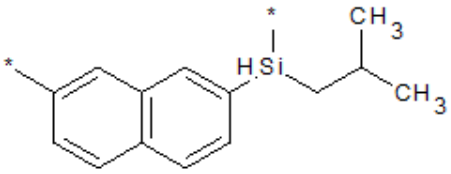
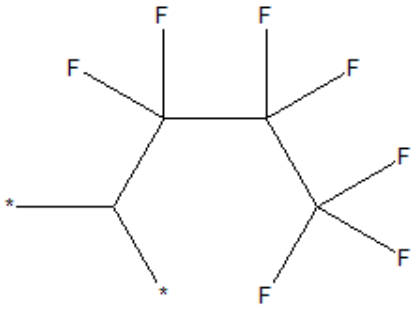
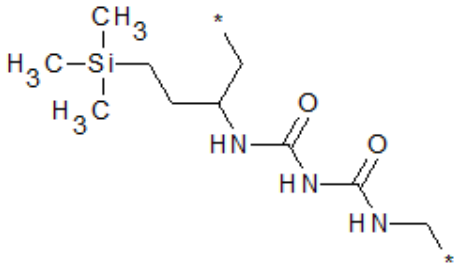
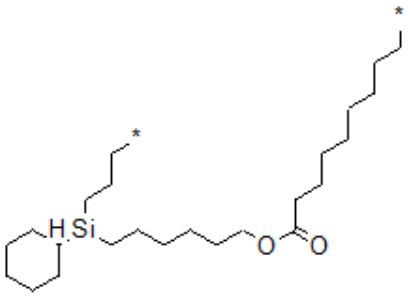
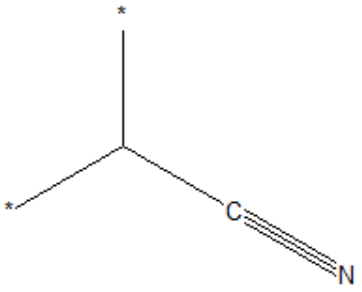
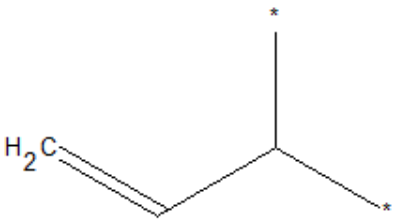
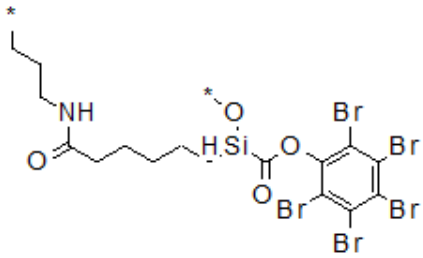
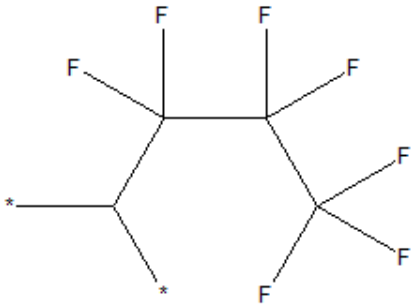
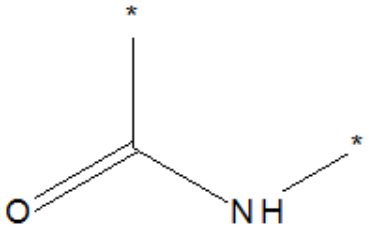
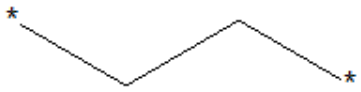
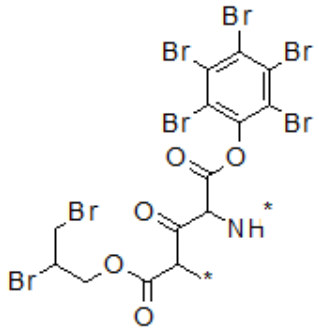
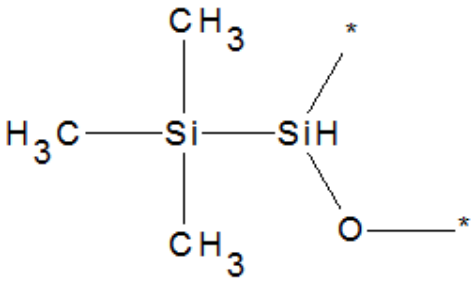
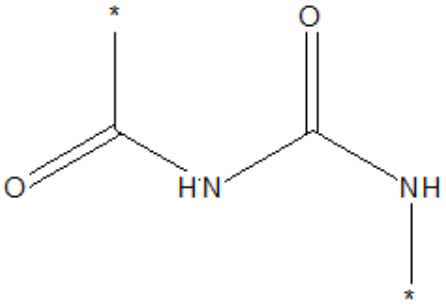
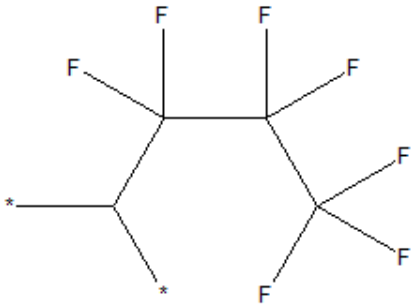
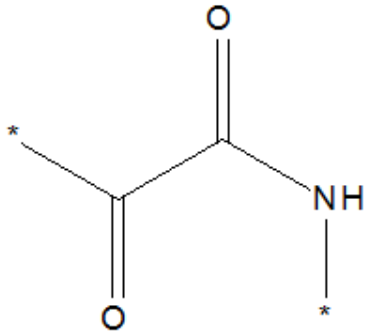
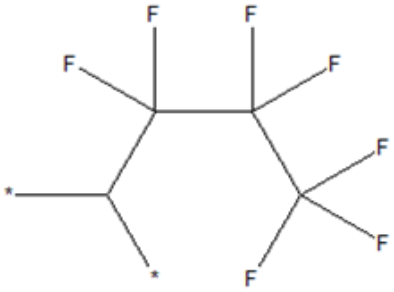
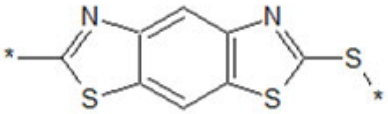
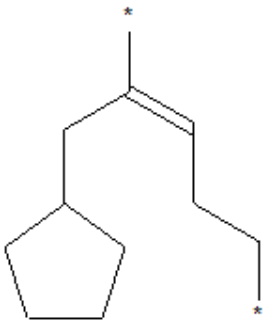
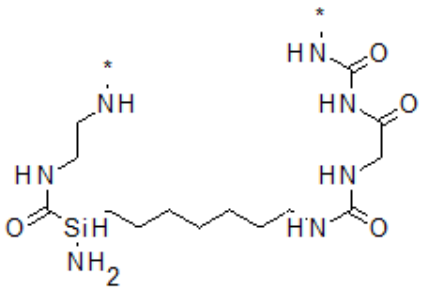
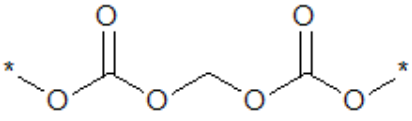
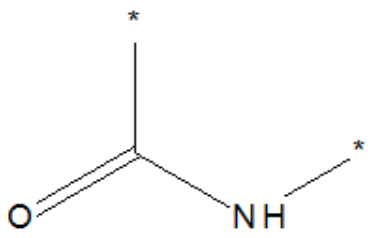
Property name	Minimal value	Maximal value
SINF MPa		
	7.082	894.4
SIGMAF MPa		
	4.055E-5	862.2
SIGMAY MPa		
	4.139	673.4

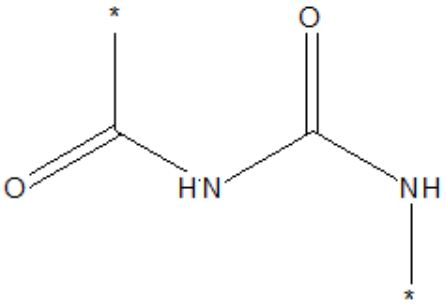
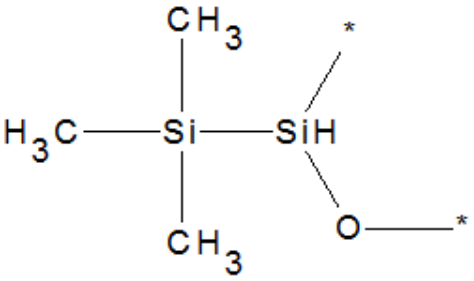
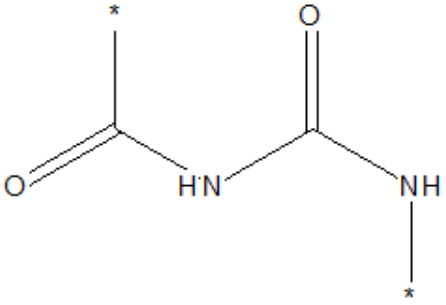
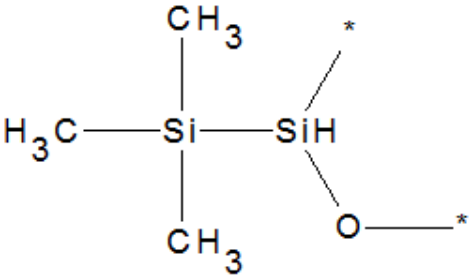
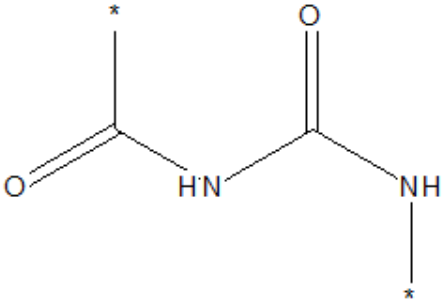
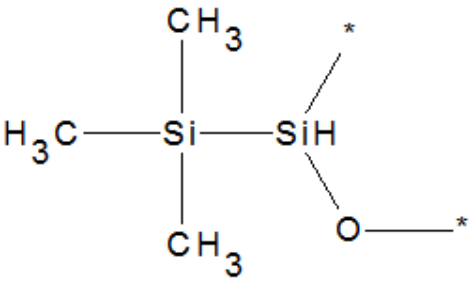
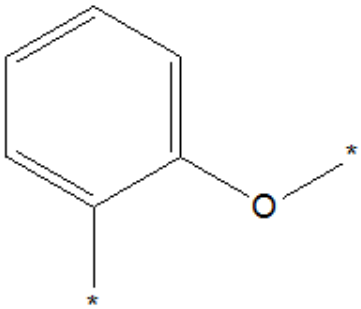
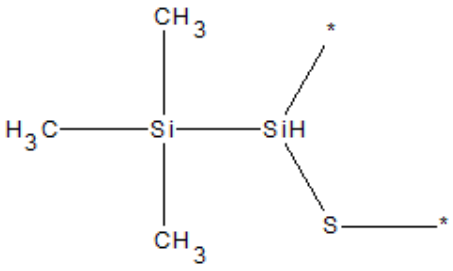
Table S7. Chemical structures with extreme property values in the MonteCarlo database.

Property name	Minimal value	Maximal value
CL J/g/K		
	0.8326	2.257
CS J/g/K		
	0.5450	1.830
COH1 J/g		
	165.3	1.321E+3

Property name	Minimal value	Maximal value
COH2 J/g		
	86.02	1.296E+3
RLL cm^3/g		
	0.1074	0.3486
PLL cm^3/g		
	0.1379	0.4842
EAFLOW kJ/g		
	4.597E-2	10.97

Property name	Minimal value	Maximal value
STIFFNESS $g^{0.25}cm^{1.5}/mole^{0.75}$		
	6.719	226.3
EPSILON		
	2.110	9.404
VISCFUNC $g^{*}J^{1/3*}mole^{-4/3}$		
	785.4	3.744E+4
DELTA1 $(J/cc)^{0.5}$		
	13.80	47.21

Property name	Minimal value	Maximal value
DELTA2 $(J/cc)^{0.5}$		
	12.98	44.12
N		
MU Debye		
	0.000	1.964
MB MPa		
	207.3	2.355E+4

Property name	Minimal value	Maximal value
O2PERM Barrers		
	5.798E-15	90.05
N2PERM Barrers		
	1.074E-16	33.35
CO2PERM Barrers		
	1.429E-15	618.6
TDECOMPK		
	368.9	1.155E+3

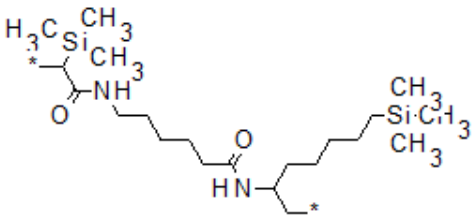
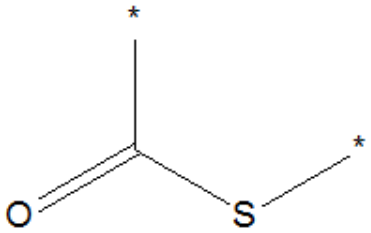
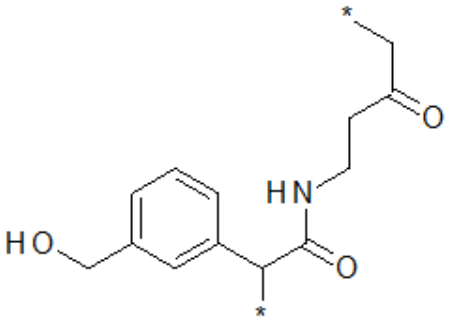
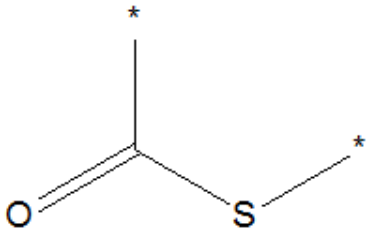
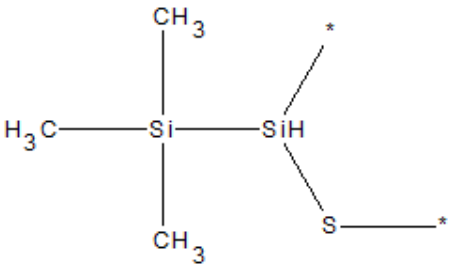
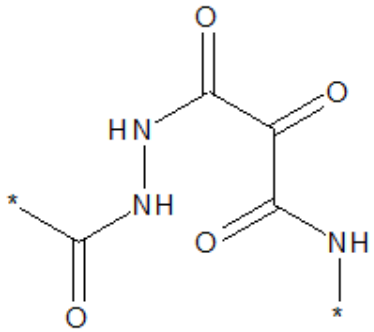
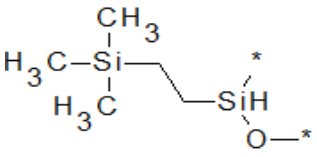
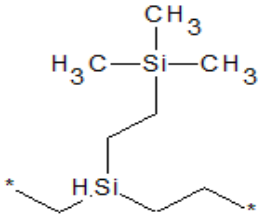
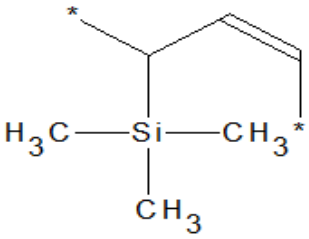
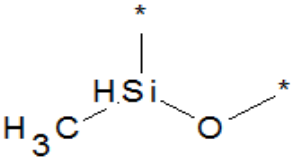
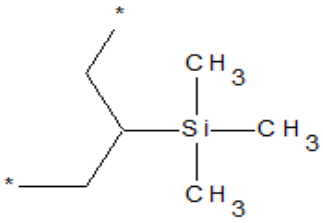
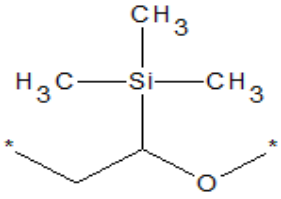
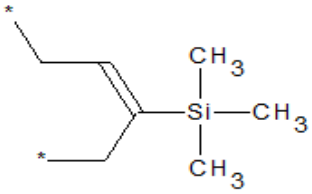
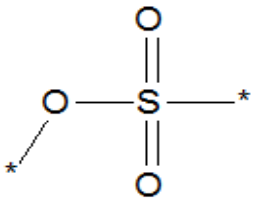
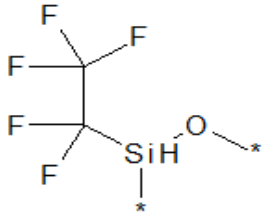
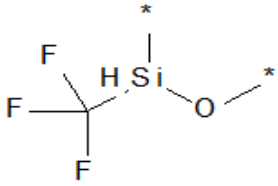
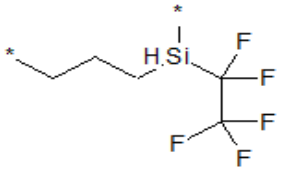
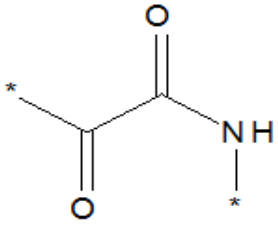
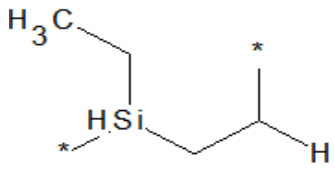
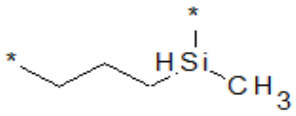
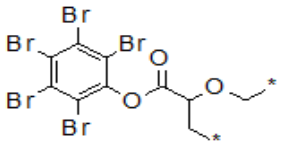
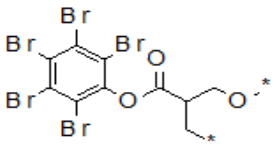
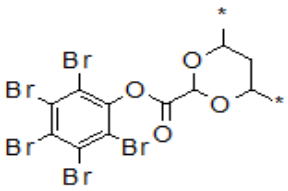
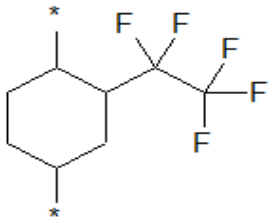
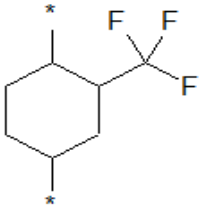
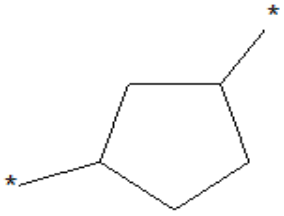
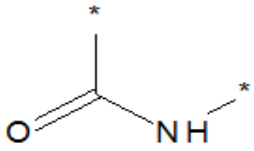
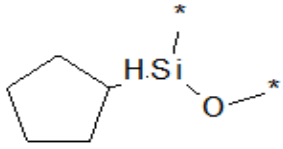
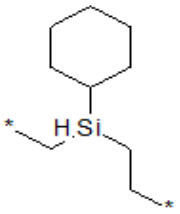
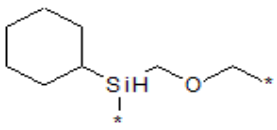
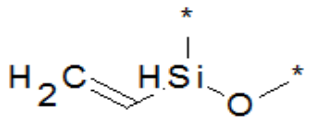
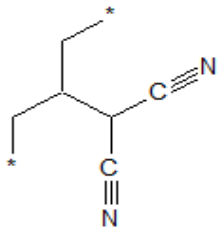
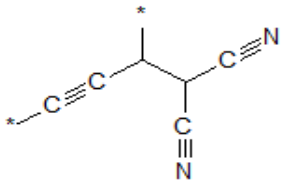
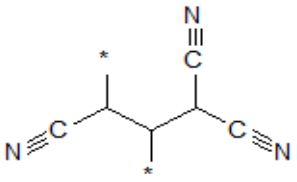
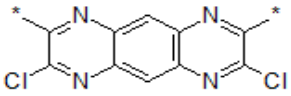
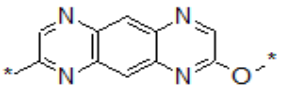
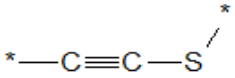
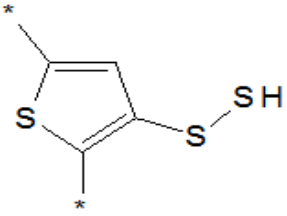
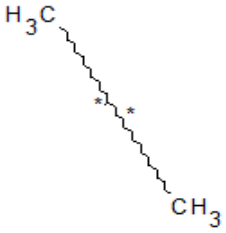
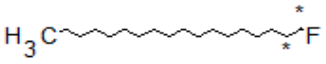
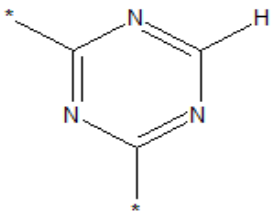
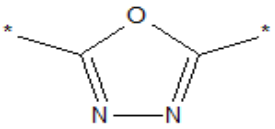
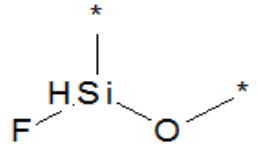
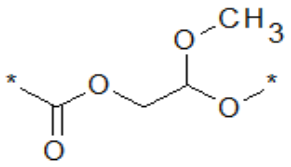
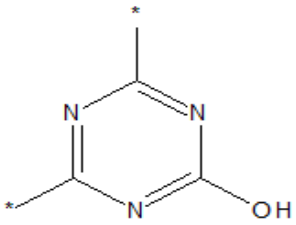
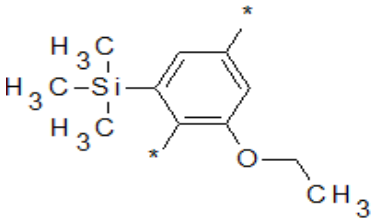
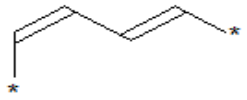
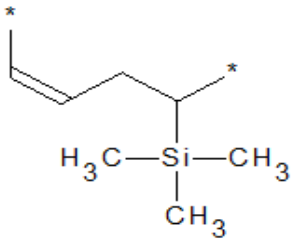
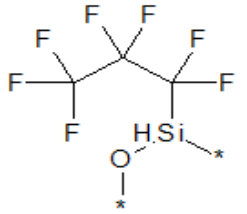
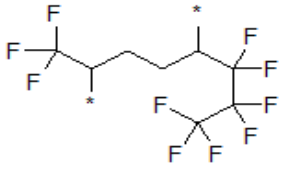
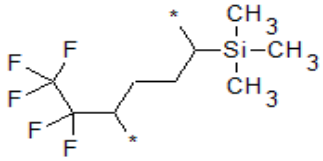
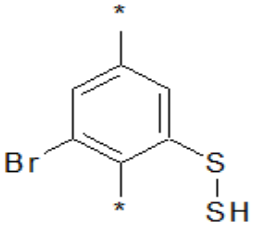
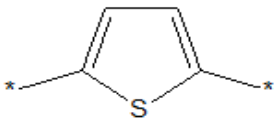
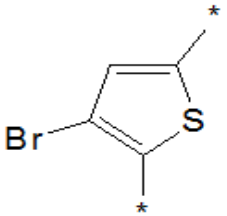
Property name	Minimal value	Maximal value
SINF MPa		
	6.548	2.424E+3
SIGMAF MPa		
	4.365E-3	2.339E+3
SIGMAY MPa		
	4.248	620.1

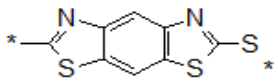
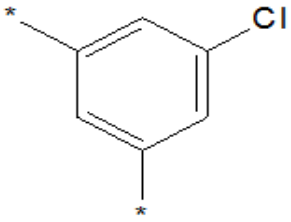
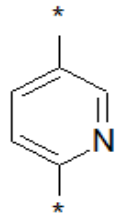
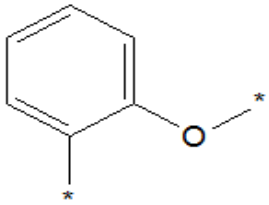
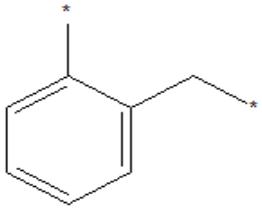
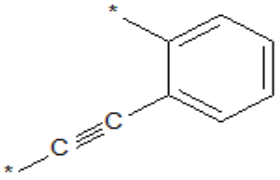
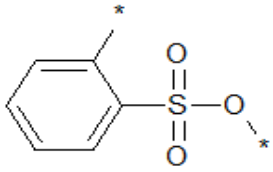
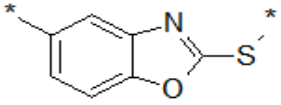
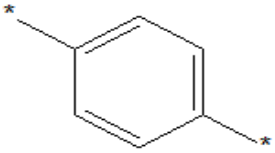
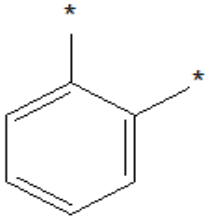
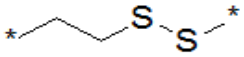
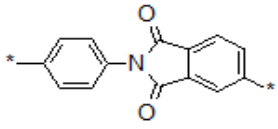
Table S8. Chemist-selected chemical structures with extreme property values from the MonteCarloAll database [53].

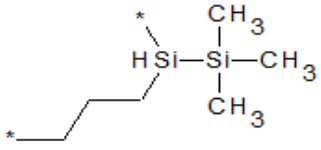
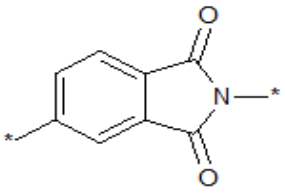
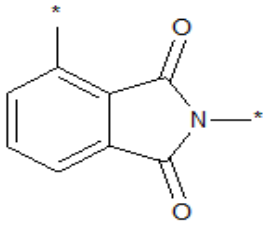
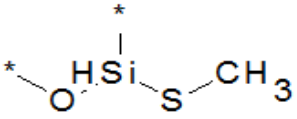
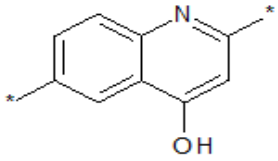
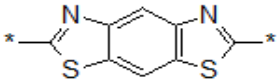
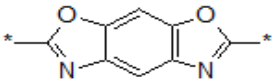
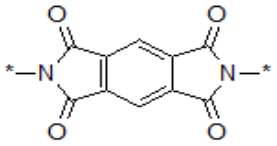
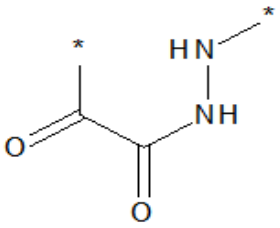
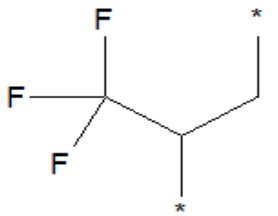
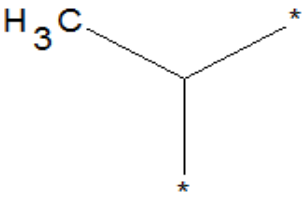
Structure	Extremal properties	Structure	Extremal properties
	DELTA1: 14.5543 $(J/cc)^{0.5}$		DELTA1: 14.6953 $(J/cc)^{0.5}$
	DELTA1: 14.7047 $(J/cc)^{0.5}$ O2PERM: 67.975 Barrers		DELTA1: 14.8919 $(J/cc)^{0.5}$ O2PERM: 46.216 Barrers
	DELTA1: 14.9043 $(J/cc)^{0.5}$ D: 0.82716		DELTA1: 14.9186 $(J/cc)^{0.5}$
	DELTA1: 14.995 $(J/cc)^{0.5}$		DELTA1: 36.584 $(J/cc)^{0.5}$ DELTA2: 37.171 $(J/cc)^{0.5}$ D: 2.50975 EPSILON: 8.095 H2OPERM: 5.030530E+0014 Barrers SIGMAFINF: 1104.55 MPa
	DELTA2: 13.2832 $(J/cc)^{0.5}$		DELTA2: 13.52 $(J/cc)^{0.5}$
	DELTA2: 13.7036 $(J/cc)^{0.5}$		DELTA2: 44.125 $(J/cc)^{0.5}$ MB: 17918.3 MPa O2PERM: 0.00000000077548 Barrers

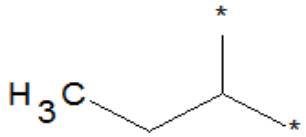
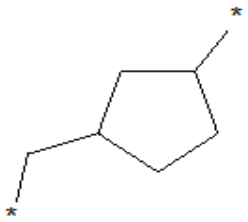
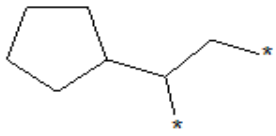
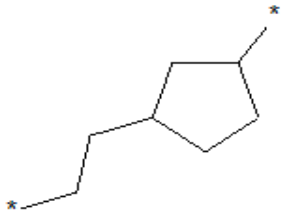
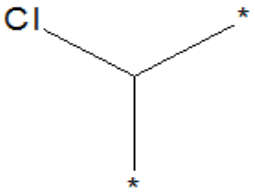
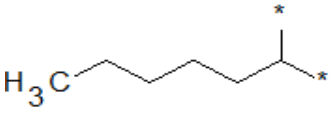
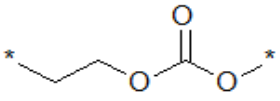
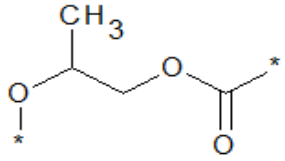
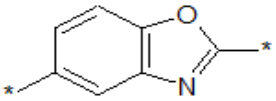
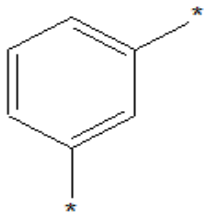
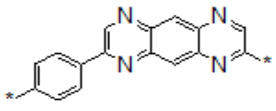
Structure	Extremal properties	Structure	Extremal properties
	D: 0.81959		D: 0.82351
	D: 2.26062		D: 2.26815
	D: 2.274		EPSILON: 2.12568
	EPSILON: 2.13343		EPSILON: 2.13435
	EPSILON: 9.4044		EAFLOW: 8.0184 kJ/g
	EAFLOW: 10.5304 kJ/g		EAFLOW: 10.8874 kJ/g

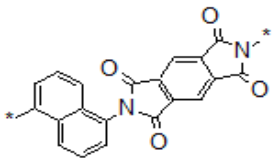
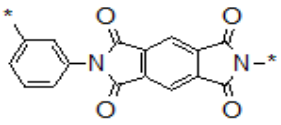
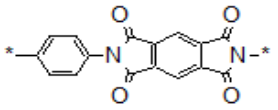
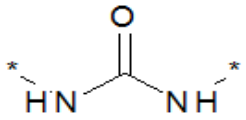
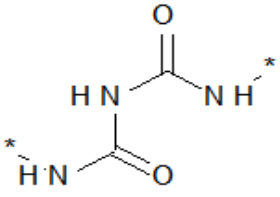
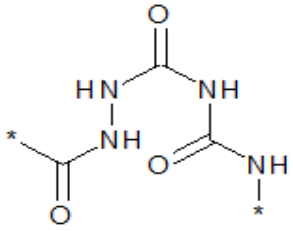
Structure	Extremal properties	Structure	Extremal properties
	EAFLOW: 10.9374 kJ/g		EAFLOW: 308.442 kJ/g
	EAFLOW: 367.45 kJ/g		EAFLOW: 505.3 kJ/g
	H2OPERM: 0.682 TGINF: 779.43		H2OPERM: 2.4303
	H2OPERM: 3.407050E+0015		H2OPERM: 2.91E+0016 N: 1.79762
	HEATCOND: 0.115001		HEATCOND: 0.115058
	HEATCOND: 0.250229		HEATCOND: 0.263205

Structure	Extremal properties	Structure	Extremal properties
	MB: 558.62 MPa O2PERM: 61.211 Barrers		MB: 614.12 MPa
	MB: 14023.9 MPa O2PERM: 0.0000000028 Barrers		O2PERM: 33.611 Barrers
	O2PERM: 37.476 Barrers		O2PERM: 49.751 Barrers
	N: 1.35309		N: 1.35751
	N: 1.36293		N: 1.74704
	N: 1.74928 SIGMAFINF: 569.56 MPa		N: 1.78785

Structure	Extremal properties	Structure	Extremal properties
	N: 1.8255		SIGMAFINF: 552.31 MPa
	SIGMAFINF: 1380.62 MPa		TDECOMP: 368.88 K
	TDECOMP: 387.81 K		TDECOMP: 438.03 K
	TDECOMP: 447.15 K		TDECOMP: 934.69 K
	TDECOMP: 938.09 K		TDECOMP: 938.87 K
	TDECOMP: 940.57 K		TDECOMP: 964.43 K

Structure	Extremal properties	Structure	Extremal properties
	TDECOMP: 973.79 K		TDECOMP: 978.24 K
	TDECOMP: 978.65 K		TDECOMP: 986.48 K
	TGINF: 721.3		
	TGINF: 791.88		TGINF: 792.82
	TGINF: 838.88		DELTA1: 37.309 $(J/cc)^{0.5}$ DELTA2: 41.32 $(J/cc)^{0.5}$ MB: 15329 MPa O2PERM: 0.0000000146236 Barrers
	DELTA2: 14.3563 $(J/cc)^{0.5}$ N: 1.36901		D: 0.84554

Structure	Extremal properties	Structure	Extremal properties
	D: 0.8457		EPSILON: 2.16868 EAFLOW: 13.4684 kJ/g
	EAFLOW: 14.5363 kJ/g		EAFLOW: 14.5363 kJ/g
	H2OPERM: 1.75037 Barrers TDECOMP: 449.56 K		HEATCOND: 0.114502
	HEATCOND: 0.115507		MB: 524.99 MPa
	MB: 668.09 MPa		TDECOMP: 934.36 K
	TDECOMP: 938.09 K		TGINF: 721.22

Structure	Extremal properties	Structure	Extremal properties
	TGINF: 724.48		TGINF: 752.53
	TGINF: 778.54		EPSILON: 7.8336
	EPSILON: 8.042		EPSILON: 8.1239