Electronic Supplementary Material (ESI) for RSC Advances.

Thermal stabilities and conformational behaviors of isocyanurates and cyclotrimerization energies of isocyanates：a computational study

Tadafumi Uchimaru,[a] Shogo Yamane,[a] Junji Mizukado,[a] and Seiji Tsuzuki[b]

[a]*Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology, Higashi, 1-1-1, Tsukuba, Ibaraki 305-8565 Japan*

[b]*Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology, Umezono, 1-1-1, Tsukuba, Ibaraki 305-8568 Japan*

Supplementary Information

- Estimation of the cyclotrimerization energy of methyl isocyanate by using thermochemical data known in the literature
- Table S1 Calculated values for CH_3−NCO bond dissociation enthalpy at 0 K and the estimates for the enthalpy of formation of methyl isocyanate at 298 K
- Table S2. Results of composite method calculations for the enthalpy values (in au) for CH_3−NCO molecule and NCO and CH_3 radicals at 0 K and 298 K
- Table S3 Extrapolation of the ROCCSD(T) single point energies of CH_3NCO molecule and NCO and CH_3 radicals to the basis set limit: estimation of the CH_3−NCO bond dissociation enthalpy
- Table S4 Extrapolation of the UCCSD(T) single point energies of CH_3NCO molecule and NCO and CH_3 radicals to the basis set limit: estimation of the CH_3−NCO bond dissociation enthalpy
- Estimation of the cyclotrimerization energy of methyl isocyanate at the CCSD(T) basis set limit value
- Table S5 Single point energies of trimethyl isocyanurate and methyl isocyanate calculated with the aug-cc-pVXZ (X = D, T, Q) basis set: Estimate for the cyclotrimerization energy at the CCSD(T) basis set limit
- Table S6 Calculated energy differences between the extreme conformers of tri-*n*-alkyl isocyanurates
- NBO analysis for the resonance stabilization energies in the isocyanate and isocyanurate molecules
- Table S7 Resonance stabilization energies in isocyanate and isocyanurate molecules
- Figure S1 Structures of tri-*n*-hexyl and tri-*n*-octyl isocyanurate
- Figure S2 Optimized structures of isocyanate molecules
- The Cartesian coordinates of the optimized isocyanurates
- The Cartesian coordinates of the optimized isocyanates

Estimation of the cyclotrimerization energy of methyl isocyanate by using thermochemical data known in the literature

We made estimation of the cyclotrimerization energy of methyl isocyanate by using thermochemical data known in the literature. Imamura et al. reported enthalpy of formation of trimethyl isocyanurate ΔH_f at 298 K as −141.1 ± 0.4 kcal/mol (−590.5 ± 1.6 kJ/mol).[1] Although no literature thermochemical data is available for methyl isocyanate, the enthalpies of formation of NCO and CH_3 radicals have been reported. The reported values of ΔH_f at 0 K values of NCO and CH_3 radicals are 30.5 kcal/mol and 35.9 ± 0.1 kcal/mol (150.3 ± 0.4 kJ/mol), respectively.[2,3] We employed high level *ab initio* methods for computing the bond dissociation energy (BDE) of CH_3−NCO. The *ab initio* derived BDE value and the literature values of the enthalpies of formation (ΔH_f) of the radicals enabled us to calculate the enthalpy of methyl isocyanate. Furthermore, by referring to the literature value for the enthalpy of formation of trimethyl isocyanurate, the cyclotrimerization enthalpy value of methyl isocyanate was obtained.

The composite *ab initio* procedures, such as CBS-APNO,[4] G3,[5] G4MP2,[6]and G4[7] methods, were employed for the computations of the CH_3−NCO BDE and the corresponding estimates of enthalpy formation of methyl isocyanate (See Tables S1 and S2). Recent extensive benchmark results show that these composite procedures provide highly accurate thermochemical values for molecules[8] and radicals.[9]

The CH_3−NCO BDE was also evaluated by applying the CCSD(T) energy assessments using the correlation consistent basis sets (aug-cc-pVXZ, X = D, T, Q, 5).[10] The single point energies of CH_3NCO, NCO, and CH_3 are collected in Tables S3 and S4. Table S3 shows the ROCCSD(T) calculated values, whereas Table S4 shows UCCSD(T) calculated values. By using the two-point extrapolation schemes, we obtained the basis set limit values of the electronic energies at the CCSD(T) level, *i. e.* $E_{\text{CCSDT (limit)}}$. For the HF energy extrapolation, the procedure prescribed by Halkier et al.[7,11] was employed. Namely,

$$E_{HF(limit)}(X, X+1) = \frac{E_{HF(X+1)} - E_{HF(X)} exp(-\alpha)}{1 - exp(-\alpha)}$$

where α=1.63. Meanwhile, the correlation energies at the CCSD(T) level were extrapolated according to the procedure reported by Helgaker et al.[12] Namely,

$$E_{CCSDT\ cor.(limit)}(X, X+1) = \frac{(X+1)^3 E_{CCSDT\ cor.\ (X+1)} - X^3 E_{CCSDT\ cor.(X)}}{(X+1)^3 - X^3}$$

The values of $E_{\text{CCSDT (limit)}}$ were obtained with the following equation.

$$E_{CCSDT(limit)} = E_{HF(limit)}(X, X+1) + E_{CCSDT\ cor.(limit)}(X, X+1)$$

The single point energies calculated with the basis sets of aug-cc-pVQZ and aug-cc-pV5Z were employed for the extrapolation to the basis set limit. That is, X = 4 for the above equations in

the present case. The same procedure was applied for the results shown in Tables S3 and S4. The $E_{CCSDT\ (limit)}$ values obtained from Tables S3 and S4 are almost identical. Table S1 shows the result obtained from the extrapolation of ROCCSD(T) single point energies given in Table S3.

These computational methods suggested us CH_3−NCO BDE values at 0 K ranging from 88 and 91 kcal/mol (Table S1). Based on these values, the enthalpy of formation ΔH_f of methyl isocyanate at 298 K was estimated to be in the range from −24 to −26 kcal/mol (Table S1). Referring to the enthalpy of formation of trimethyl isocyanurate, the cyclotrimerization enthalpy of methyl isocyanate was estimated to be between −62 and −70 kcal/mol.

Table S1 Calculated values for CH_3−NCO bond dissociation enthalpy at 0 K and the estimates for the enthalpy of formation of methyl isocyanate at 298 K

Computational method	$BDE_{0\ K}$[a]	$\Delta H_{f\ 298\ K}$[a,b]
CBS-APNO	89.7	−25.3
G3	87.9	−23.5
G4MP2	88.2	−23.8
G4	88.5	−24.1
Basis set limit value at the CCSD(T) level[c]	90.9	−26.4

[a] See the text.

[b] According to the procedure prescribed by Curtiss et al.,[13] the values of $\Delta H_{f\ 298K}$ were derived from those of $\Delta H_{f\ 0K}$.

[c] See Tables S3.

Table S2. Results of composite method calculations for the enthalpy values (in au) for CH_3−NCO molecule and NCO and CH_3 radicals at 0 K and 298 K

Computational method	Temperarure	CH_3−NCO	NCO	CH_3
CBS-APNO	0 K	-207.931424	-167.984792	-39.803682
	298 K	-207.925719	-167.981124	-39.799526
G3	0 K	-207.854151	-167.920789	-39.793292
	298 K	-207.848367	-167.917060	-39.789046
G4MP2	0 K	-207.728638	-167.826662	-39.761454
	298 K	-207.722949	-167.822973	-39.757408
G4	0 K	-207.891750	-167.950718	-39.799954
	298 K	-207.886061	-167.947028	-39.795909

Table S3 Extrapolation of the ROCCSD(T) single point energies of CH_3NCO molecule and NCO and CH_3 radicals to the basis set limit: estimation of the CH_3−NCO bond dissociation enthalpy[a]

		CH_3NCO	NCO	CH_3	BDE_e (kcal/mol)	BDE_0 (kcal/mol)
ZPE		0.050099	0.011132	0.029594		
Basis set	Computational level					
aug-cc-pVDZ	HF	-206.818612	-167.145021	-39.561662		
	CCSDT	-207.496886	-167.627183	-39.724163	91.328	
	E_{corr}	-0.678274	-0.482162	-0.162501		
aug-cc-pVTZ	HF	-206.869569	-167.183126	-39.573498		
	CCSDT	-207.676651	-167.761606	-39.763629	95.015	
	E_{corr}	-0.807082	-0.578480	-0.190131		
aug-cc-pVQZ	HF	-206.882487	-167.193589	-39.575897		
	CCSDT	-207.729380	-167.802743	-39.773318	96.209	
	E_{corr}	-0.846893	-0.609154	-0.197421		
aug-cc-pV5Z	HF	-206.885366	-167.195849	-39.576516		
	CCSDT	-207.745594	-167.815679	-39.776129	96.502	
	E_{corr}	-0.860228	-0.619830	-0.199613		
HF_{limit}		-206.886068	-167.196400	-39.576667		
$E_{corr\ limit}$		-0.874219	-0.631031	-0.201913		
$E_{CCSDT\ limit}$		-207.760286	-167.827431	-39.778580	96.810	
E_0		-207.710187	-167.816299	-39.748986		90.928

[a] Geometry optimizations were carried out at the MP2/6-311+G(2df,p) level. The zero point energies were computed using scale factor of 0.9777 prescribed by Merrick et al.[14]

Table S4 Extrapolation of the UCCSD(T) single point energies of CH_3NCO molecule and NCO and CH_3 radicals to the basis set limit: estimation of the CH_3−NCO bond dissociation enthalpy[a]

		CH_3NCO	NCO	CH_3	BDE_e (kcal/mol)	BDE_0 (kcal/mol)
ZPE		0.050099	0.011132	0.029594		
Basis set	Computational level					
aug-cc-pVDZ	HF	-206.818612	-167.153878	-39.565801		
	CCSDT	-207.496886	-167.627020	-39.724178	91.421	
	E_{corr}	-0.678274	-0.473142	-0.158377		
aug-cc-pVTZ	HF	-206.869569	-167.192303	-39.578016		
	CCSDT	-207.676651	-167.761405	-39.763648	95.129	
	E_{corr}	-0.807082	-0.569102	-0.185632		
aug-cc-pVQZ	HF	-206.882487	-167.202825	-39.580445		
	CCSDT	-207.729380	-167.802541	-39.773339	96.323	
	E_{corr}	-0.846893	-0.599716	-0.192894		
aug-cc-pV5Z	HF	-206.885366	-167.205097	-39.581070		
	CCSDT	-207.745594	-167.815431	-39.776144	96.648	
	E_{corr}	-0.860228	-0.610334	-0.195074		
HF_{limit}		-206.886068	-167.205651	-39.581222		
$E_{corr\ limit}$		-0.874219	-0.621474	-0.197361		
$E_{CCSDT\ limit}$		-207.760286	-167.827125	-39.778584	96.999	
E_0		-207.710187	-167.815993	-39.748990		91.118

[a] Geometry optimizations were carried out at the MP2/6-311+G(2df,p) level. The zero point energies were computed using scale factor of 0.9777 prescribed by Merrick et al.[14]

Estimation of the cyclotrimerization energy of methyl isocyanate at the CCSD(T) basis set limit value

By using two-point extrapolation schemes, the HF energies and the MP2 correlation energies calculated with the basis sets of the aug-cc-pVTZ and aug-cc-pVQZ were extrapolated. For the HF energy extrapolation, we employed the procedure developed by Halkier et al.[7,11] The basis set limit energy value at the HF level $E_{\mathrm{HF(limit)}}(3, 4)$ is given by the following equation:

$$E_{HF(limit)}(3,4) = \frac{E_{HF(4)} - E_{HF(3)} exp(-\alpha)}{1 - exp(-\alpha)}$$

where α = 1.63. Meanwhile, the MP2 correlation energies were extrapolated using the procedure prescribed by Helgaker et al.[12] The MP2 correlation energy at the basis set limit $E_{\mathrm{MP2\ cor.(limit)}}$ is given by the following equation:

$$E_{MP2\ cor.\ (limit)} = \frac{4^3 E_{MP2\ cor.(4)} - 3^3 E_{MP2cor.(3)}}{4^3 - 3^3}$$

In addition, we considered values of $\Delta_{\mathrm{CCSDT}}(2)$ and γ. The former is the difference between the MP2 and CCSD(T) energies calculated with the basis set of the aug-cc-pVDZ. The latter is the ratio of the MP2 correlation energy calculated with the aug-cc-pVDZ relative to the MP2 correlation energy at the basis set limit $E_{\mathrm{MP2\ cor.(limit)}}$. Namely,

$$\Delta_{CCSDT}(2) = E_{CCSDT(2)} - E_{MP2(2)}$$

$$\gamma = E_{MP2\ cor.\ (2)} / E_{MP2\ cor.(limit)}$$

The following equation shows our estimated CCSD(T) energy value at the basis set limit, $E_{\mathrm{CCSDT(limit)}}$.

$$E_{CCSDT(limit)} = E_{HF(limit)}(3,4) + E_{MP2\ cor.(limit)} + \frac{\Delta_{CCSDT}(2)}{\gamma}$$

Through the above described procedures, we obtained an estimate for the electronic energy change upon cyclotrimerization of methyl isocyanate. Our estimated CCSD(T) energy value at the basis set limit is −71.6 kcal/mol.

Table S5 Single point energies of trimethyl isocyanurate and methyl isocyanate calculated with the aug-cc-pVXZ (X = D, T, Q) basis set: Estimate for the cyclotrimerization energy at the CCSD(T) basis set limit

Basis set (X)	Trimer (Isocyanurate)	Monomer (Isocyanate)	Cyclotrimerization energy (kcal/mol))
		HF	
D	-620.555658	-206.819741	-60.5
T	-620.701172	-206.871144	-55.1
Q	-620.739444	-206.884130	-54.6
		MP2	
D	-622.474844	-207.453549	-71.7
T	-623.008363	-207.633158	-68.3
Q	-623.181816	-207.691365	-67.6
		CCSD(T)	
D	-622.607359	-207.495947	-75.0
T			
CCSD(T)limit			-71.6
Enthalpy correction			5.1
ΔH			-66.4

Table S6 Calculated energy differences between the extreme conformers of tri-*n*-alkyl isocyanurates[a]

R	Computational level						
	B3LYP[b]	HF[b]	B3LYP-GD3[b]	B3LYP-GD3BJ[b]	MP2[b]	ONIOM(1)[c]	ONIOM(2)[d]
Me ($C_s - C_{3h}$)	0.04	0.04	0.05	0.04	0.05	0.05	0.05
Et ($C_s - C_{3v}$)	-0.06	-0.04	0.07	0.04	0.07	0.07	0.07
n-Pr ($C_s - C_3$)	-3.78	-4.59	0.07	-0.05	0.52	0.05	0.53
n-Bu ($C_s - C_3$)	-4.43	-5.33	0.63	0.47	1.24	0.06	1.25
n-Hex ($C_s - C_3$)	-10.02	-12.75	5.57	4.92	5.08	5.61	5.12
n-Oct ($C_s - C_3$)	-11.16		9.53	8.63		9.56	

[a] The energy differences between the conformers calculated with taking the BSSEs into account are given in kcal/mol. Positive values indicate that the conformers possessing the C_3 axis are lower in energy than the C_s isomers. The geometries of the conformers were optimized at the B3LYP-GD3/cc-pVTZ level. The BSSE-uncorrected energy differences between the conformers are given in Table 3, but almost identical results were obtained whether or not the BSSEs were taken into account.

[b] The cc-pVTZ basis set was utilized.

[c] ONIOM(CCSD(T)/cc-pVTZ:B3LYP-GD3/cc-pVTZ)

[d] ONIOM(CCSD(T)/cc-pVTZ:MP2/cc-pVTZ)

NBO analysis for the resonance stabilization energies in the isocyanate and isocyanurate molecules

The NBO analysis was applied to examine the differences in the resonance orbital interactions between the trialkyl isocyanates and the phenyl substituted analogue. The NBO program version 6.0[15] implemented in the Gaussian 09 was employed. There have been reported criticisms that the second order perturbation theory in the NBO analysis tends to overestimate the resonance energies.[16,17] However, the NBO analysis would be helpful in obtaining at least qualitatively correct pictures or trends.

Table S7 shows the calculated resonance stabilization energies due to the orbital interactions between the substituents and the NCO moiety in the isocyanate molecules. In addition, those between the substituents and the isocyanate ring in the isocyanurate molecules are also shown in Table S7. The resonance stabilization energy was found to be considerably smaller for triphenyl isocyanurate than for phenyl isocyanate. Namely, for the phenyl derivative, the resonance stabilization energy will be reduced upon the cyclotrimerization. For the alkyl-substituted derivatives, the degree of the change in the resonance stabilization upon cyclotrimerization was indicated to be relatively smaller than for the phenyl derivative. These differences between phenyl and alkyl derivatives are inferred as the main cause of the difference in trend between these two types of derivatives seen in Figure 4b.

Table S7 Resonance stabilization energies in isocyanate and isocyanurate molecules[a]

R		*R* → NCO/ICN[b]	*R* ← NCO/ICN[c]	*R* ⇆ NCO/ICN[d]
Me	R─N=C=O	16.0	23.0	38.4
	isocyanurate	16.2	18.9	35.0
	Δ[e]	0.2	-4.1	-3.4
n-Oct	R─N=C=O	17.2	25.1	41.6
	isocyanurate	18.7	22.6	41.0
	Δ[e]	1.5	-2.5	-0.6
Ph	R─N=C=O	20.8	38.9	58.0
	isocyanurate	20.7	29.5	49.7
	Δ[e]	-0.1	-9.4	-8.3

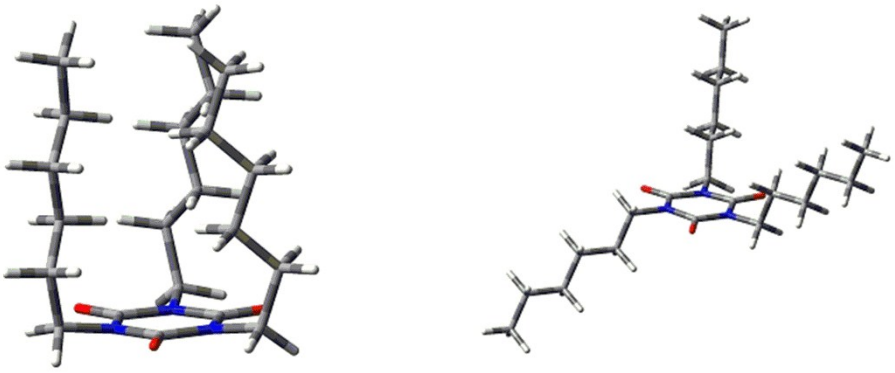
[a] The resonance stabilization energies were evaluated with the second order perturbation theory. The abbreviation of ICN stands for the isocyanurate ring. Energy values are given in kcal/mol.

[b] The stabilization energies due to the resonance interactions between the bonding orbitals in the substituent and the anti-bonding orbitals of NCO moiety or isocyanurate ring.

[c] The stabilization energies due to the resonance interactions between the anti-bonding orbitals in the substituent and the bonding orbitals of NCO moiety or isocyanurate ring.

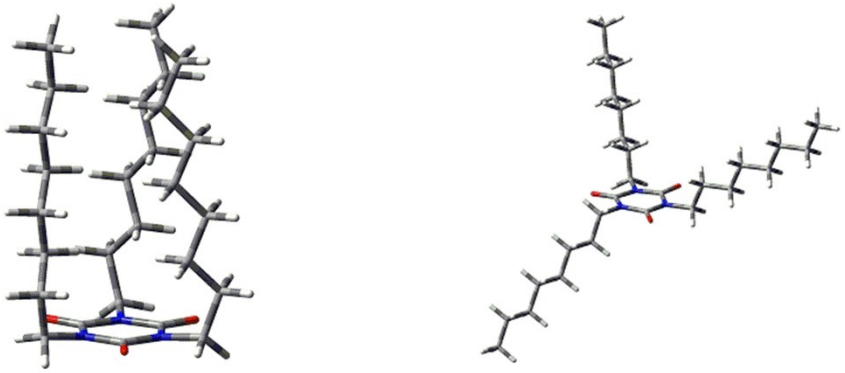
[d] The stabilization energies due to the resonance interactions between the orbitals in the substituent and those of NCO moiety or isocyanurate ring.

[e] The difference between the isocyanate and isocyanurate molecules.



C_3 C_s

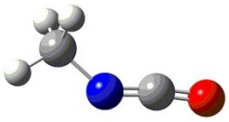
Tri-*n*-hexyl isocyanurate



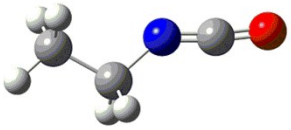
C_3 C_s

Tri-*n*-octyl isocyanurate

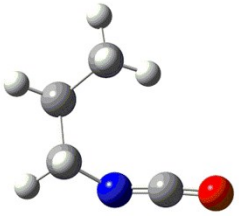
Figure S1 Structures of tri-*n*-hexyl and tri-*n*-octyl isocyanurate



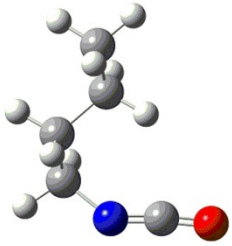
Me-NCO (C_s)



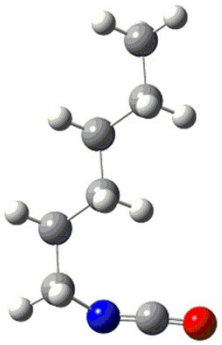
Et-NCO (C_s)



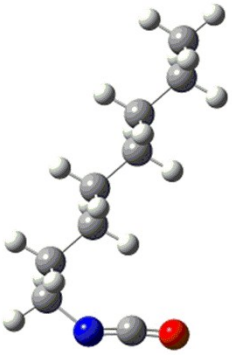
n-Pr-NCO (C_1)



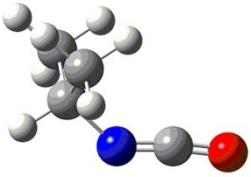
n-Bu-NCO (C_1)



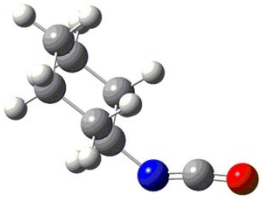
n-Hex-NCO (C_1)



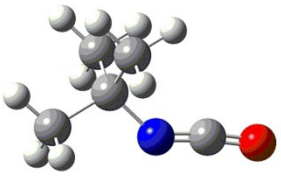
n-Oct-NCO (C_1)



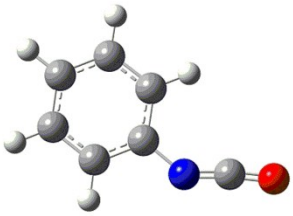
i-Pr-NCO (C_s)



Cy-NCO (C_s)



t-Bu-NCO (C_s)



Ph-NCO (C_s)

Figure 2S Optimized structures of isocyanate molecules

References

1 A. Imamura, K. Takahashi, S. Murata and M. Sakiyama, *J. Chem. Thermodynamics,* 1989, **21**, 237-246.

2 Y. Ji, P. Bobadova-Parvanova, C. Larson, P. C. Samartis, K. Morokuma, J. J-M. Lin, T.-T. Ching, C. Chaudhuri, S.-H. Lee and A. M. Wodtke, *J. Chem. Phys.,* 2006, **124**, 241106.

3 E. A. Fogleman, H. Koizumi, J. P. Kercher, B. Sztáray and T. Baer, *J. Phys. Chem. A,* 2004, **108**, 5288-5294.

4 J. W. Ochterski, G. A. Petersson and J. A. Montgomery Jr., *J. Chem. Phys.,* 1996, **104**, 2598-2619.

5 L. A. Curtiss, K. Raghavachari, P. C. Redfern, V. Rassolve and J. A. Pople, *J. Chem. Phys.,* 1998, **109**, 7764-7776.

6 L. A. Curtiss, P. C. Redfern and K. Raghavachari, *J. Chem. Phys.,* 2007, **127**, 124105.

7 L. A. Curtiss, P. C. Redfern and K. Raghavachari, *J. Chem. Phys.,* 2007, **126**, 084108.

8 J. M. Simmie and K. P. Somers, *J. Phys. Chem. A,* 2015, **119**, 7235-7246.

9 K. P. Somers and J. M. Simmie, *J. Phys. Chem. A,* 2015, **119**, 8922-8933.

10 a) T. H. Dunning Jr., *J. Chem. Phys.* 1989, **90**, 1007-1023; b) R. A. Kendall and T. H. Dunning Jr., *J. Chem. Phys.,* 1992, **96**, 6796-6806.

11 A. Halkier, T. Helgaker, P. Jørgensen, W. Klopper and J. Olsen, *Chem. Phys. Lett.,* 1999, **302**, 437-446.

12 T. Helgaker, W. Klopper, H. Koch and J. Noga, *J. Chem. Phys.,* 1997, **106**, 9639-9646.

13 L. A. Curtiss, K. Raghavachari, P. C. Redfern and J. A. Pople, *J. Chem. Phys.,* 1997, **106**, 1063-1079.

14 J. P. Merrick, D. Moran and L. Radom, *J. Chem. Phys. A,* 2007, **111**, 11683-11700.

15 E. D. Glendening, C. R. Landis and F. Weinhold, *J. Comput. Chem.,* 2013, **34**, 1429-1437.

16 S. Karthikeyan, R. Dedlak and P. Hobza, *J. Phys. Chem. A,* 2011, **115**, 9422-9428.

17 A. J. Stone, *J. Phys. Chem. A,* 2017, **121**, 1531-1534.

The Cartesian coordinates of the optimized isocyanurates

Trimethyl isocyanurate (C_{3h}) (RB3LYP) = -624.312105020

1	6	0	-1.229136	0.711057	0.000000
2	7	0	0.000000	1.356441	0.000000
3	6	0	1.230361	0.708935	0.000000
4	7	0	1.174712	-0.678221	0.000000
5	6	0	-0.001225	-1.419991	0.000000
6	7	0	-1.174712	-0.678221	0.000000
7	8	0	-2.269391	1.332034	0.000000
8	8	0	2.288271	1.299333	0.000000
9	8	0	-0.018880	-2.631367	0.000000
10	6	0	-2.428207	-1.439769	0.000000
11	6	0	-0.032773	2.822773	0.000000
12	6	0	2.460980	-1.383004	0.000000
13	1	0	-2.471544	-2.073635	0.882525
14	1	0	-3.247410	-0.731471	0.000000
15	1	0	-2.471544	-2.073635	-0.882525
16	1	0	-0.560049	3.177238	0.882525
17	1	0	0.990232	3.178075	0.000000
18	1	0	-0.560049	3.177238	-0.882525
19	1	0	3.031593	-1.103602	-0.882525
20	1	0	3.031593	-1.103602	0.882525
21	1	0	2.257178	-2.446604	0.000000

Trimethyl isocyanurate (C_s) E(RB3LYP) = -624.312027966

1	6	0	0.005570	-1.432099	0.000000
2	7	0	-1.169263	-0.687796	0.000000
3	6	0	-1.222255	0.699122	0.000000
4	7	0	0.000000	1.354345	0.000000
5	6	0	1.230181	0.708856	0.000000
6	7	0	1.176373	-0.679477	0.000000
7	8	0	0.009608	-2.643422	0.000000
8	8	0	-2.273706	1.301211	0.000000
9	8	0	2.287453	1.300372	0.000000
10	6	0	2.467718	-1.376359	0.000000
11	6	0	-2.458345	-1.387694	0.000000
12	6	0	-0.040611	2.819927	0.000000
13	1	0	3.036334	-1.092669	0.882416
14	1	0	2.271793	-2.441199	0.000000
15	1	0	3.036334	-1.092669	-0.882416
16	1	0	-3.027722	-1.105344	-0.882437
17	1	0	-2.259920	-2.452136	0.000000
18	1	0	-3.027722	-1.105344	0.882437
19	1	0	-0.569858	3.171560	-0.882563
20	1	0	-0.569858	3.171560	0.882563
21	1	0	0.980464	3.180934	0.000000

Triethyl isocyanurate (C_{3v}) E(RB3LYP) = -742.315946725

1	7	0	-1.175428	0.678634	-0.384166
2	6	0	0.000000	1.418165	-0.351957
3	7	0	1.175428	0.678634	-0.384166
4	6	0	1.228167	-0.709082	-0.351957
5	7	0	0.000000	-1.357268	-0.384166
6	6	0	-1.228167	-0.709082	-0.351957
7	8	0	0.000000	2.629876	-0.300934
8	8	0	2.277540	-1.314938	-0.300934
9	8	0	-2.277540	-1.314938	-0.300934
10	6	0	-2.903434	1.676298	1.097765
11	6	0	-2.452811	1.416131	-0.333168
12	6	0	2.903434	1.676298	1.097765
13	6	0	2.452811	1.416131	-0.333168
14	6	0	0.000000	-3.352597	1.097765
15	6	0	0.000000	-2.832262	-0.333168
16	1	0	-3.847765	2.221508	1.096564
17	1	0	-3.053296	0.736785	1.628755
18	1	0	-2.164723	2.275840	1.628755
19	1	0	-2.296109	2.348619	-0.866643
20	1	0	-3.182018	0.814180	-0.866643
21	1	0	3.847765	2.221508	1.096564
22	1	0	2.164723	2.275840	1.628755
23	1	0	3.053296	0.736785	1.628755

24	1	0	3.182018	0.814180	-0.866643
25	1	0	2.296109	2.348619	-0.866643
26	1	0	0.000000	-4.443017	1.096564
27	1	0	0.888573	-3.012625	1.628755
28	1	0	-0.888573	-3.012625	1.628755
29	1	0	-0.885909	-3.162798	-0.866643
30	1	0	0.885909	-3.162798	-0.866643

Triethyl isocyanurate (C_s) E(RB3LYP) = -742.315835805

1	7	0	-0.307644	-0.629233	1.175154
2	6	0	0.046153	0.712978	1.228512
3	7	0	0.237966	1.332361	0.000000
4	6	0	0.046153	0.712978	-1.228512
5	7	0	-0.307644	-0.629233	-1.175154
6	6	0	-0.438089	-1.358250	0.000000
7	8	0	0.185410	1.303335	2.278738
8	8	0	0.185410	1.303335	-2.278738
9	8	0	-0.666814	-2.549233	0.000000
10	6	0	0.851523	-1.935647	2.942887
11	6	0	-0.465911	-1.350166	2.453168
12	6	0	-0.623757	3.662680	0.000000
13	6	0	0.603930	2.762159	0.000000
14	6	0	0.851523	-1.935647	-2.942887
15	6	0	-0.465911	-1.350166	-2.453168
16	1	0	0.697315	-2.459061	3.886973
17	1	0	1.246674	-2.647627	2.219010
18	1	0	1.584112	-1.145993	3.107161
19	1	0	-0.862668	-0.635320	3.167514
20	1	0	-1.198595	-2.132775	2.281751
21	1	0	-0.316918	4.709059	0.000000
22	1	0	-1.229079	3.485130	-0.888392
23	1	0	-1.229079	3.485130	0.888392
24	1	0	1.208450	2.929988	0.886040
25	1	0	1.208450	2.929988	-0.886040
26	1	0	0.697315	-2.459061	-3.886973
27	1	0	1.584112	-1.145993	-3.107161
28	1	0	1.246674	-2.647627	-2.219010
29	1	0	-1.198595	-2.132775	-2.281751
30	1	0	-0.862668	-0.635320	-3.167514

Tri-*n*-propyl isocyanurate (C_3) E(RB3LYP) = -860.309214480

1	7	0	0.093606	1.354646	-0.757531
2	6	0	-1.176283	0.792819	-0.755438
3	7	0	-1.219961	-0.596257	-0.757531
4	6	0	-0.098460	-1.415101	-0.755438
5	7	0	1.126354	-0.758388	-0.757531
6	6	0	1.274743	0.622282	-0.755438
7	8	0	-2.177090	1.477504	-0.749012
8	8	0	-0.191011	-2.624168	-0.749012
9	8	0	2.368101	1.146663	-0.749012
10	6	0	0.934452	2.858222	1.748689
11	6	0	-0.060050	3.373293	0.709526
12	6	0	0.178334	2.828124	-0.698337
13	6	0	-2.942519	-0.619851	1.748689
14	6	0	-2.891333	-1.738651	0.709526
15	6	0	-2.538394	-1.259620	-0.698337
16	6	0	2.008066	-2.238370	1.748689
17	6	0	2.951382	-1.634642	0.709526
18	6	0	2.360060	-1.568504	-0.698337
19	1	0	0.742651	3.308033	2.723067
20	1	0	0.858114	1.776087	1.869043
21	1	0	1.962012	3.081907	1.461533
22	1	0	0.000000	4.462578	0.645404
23	1	0	-1.081252	3.134284	1.009015
24	1	0	1.169469	3.091225	-1.054284
25	1	0	-0.567294	3.218911	-1.385612
26	1	0	-3.236166	-1.010862	2.723067
27	1	0	-1.967194	-0.144895	1.869043
28	1	0	-3.650016	0.158199	1.461533
29	1	0	-3.864706	-2.231289	0.645404
30	1	0	-2.173744	-2.503534	1.009015
31	1	0	-3.261814	-0.532822	-1.054284

32	1	0	-2.504012	-2.100747	-1.385612
33	1	0	2.493516	-2.297171	2.723067
34	1	0	1.109079	-1.631192	1.869043
35	1	0	1.688004	-3.240106	1.461533
36	1	0	3.864706	-2.231289	0.645404
37	1	0	3.254996	-0.630751	1.009015
38	1	0	2.092345	-2.558402	-1.054284
39	1	0	3.071306	-1.118164	-1.385612

Tri-*n*-propyl isocyanurate (C_s) E(RB3LYP) = -860.309048593

1	7	0	0.402885	-0.596426	1.175127
2	6	0	-0.018901	0.725962	1.228503
3	7	0	-0.241114	1.335018	0.000000
4	6	0	-0.018901	0.725962	-1.228503
5	7	0	0.402885	-0.596426	-1.175127
6	6	0	0.571968	-1.317412	0.000000
7	8	0	-0.188716	1.308307	2.278813
8	8	0	-0.188716	1.308307	-2.278813
9	8	0	0.863739	-2.494633	0.000000
10	6	0	-0.466314	-2.695971	4.269123
11	6	0	-0.687353	-1.965434	2.946931
12	6	0	0.596704	-1.307650	2.451279
13	6	0	0.025657	5.164278	0.000000
14	6	0	0.498441	3.712652	0.000000
15	6	0	-0.678664	2.742370	0.000000
16	6	0	-0.466314	-2.695971	-4.269123
17	6	0	-0.687353	-1.965434	-2.946931
18	6	0	0.596704	-1.307650	-2.451279
19	1	0	-1.387165	-3.163499	4.617662
20	1	0	0.286024	-3.480216	4.164653
21	1	0	-0.127092	-2.008806	5.046748
22	1	0	-1.451765	-1.195157	3.066340
23	1	0	-1.039096	-2.664069	2.185408
24	1	0	1.368586	-2.053961	2.284465
25	1	0	0.953795	-0.575844	3.170698
26	1	0	0.871149	5.852148	0.000000
27	1	0	-0.579696	5.381234	-0.882299
28	1	0	-0.579696	5.381234	0.882299
29	1	0	1.113135	3.517348	0.880834
30	1	0	1.113135	3.517348	-0.880834
31	1	0	-1.290851	2.884283	-0.886391
32	1	0	-1.290851	2.884283	0.886391
33	1	0	-1.387165	-3.163499	-4.617662
34	1	0	-0.127092	-2.008806	-5.046748
35	1	0	0.286024	-3.480216	-4.164653
36	1	0	-1.039096	-2.664069	-2.185408
37	1	0	-1.451765	-1.195157	-3.066340
38	1	0	0.953795	-0.575844	-3.170698
39	1	0	1.368586	-2.053961	-2.284465

Tri-*n*-butyl isocyanurate (C_3) E(PB3ΛΨΠ) = –978.301982362

1	7	0	0.093361	1.354448	-1.286632
2	6	0	-1.176078	0.792590	-1.282171
3	7	0	-1.219667	-0.596372	-1.286632
4	6	0	-0.098364	-1.414808	-1.282171
5	7	0	1.126306	-0.758077	-1.286632
6	6	0	1.274442	0.622218	-1.282171
7	8	0	-2.177029	1.477079	-1.268300
8	8	0	-0.190674	-2.623902	-1.268300
9	8	0	2.367702	1.146822	-1.268300
10	6	0	0.625426	3.322826	2.679441
11	6	0	0.898722	2.770727	1.281962
12	6	0	-0.071474	3.325157	0.238193
13	6	0	0.178439	2.825453	-1.184325
14	6	0	-3.190365	-1.119778	2.679441
15	6	0	-2.848881	-0.607047	1.281962
16	6	0	-2.843933	-1.724477	0.238193
17	6	0	-2.536134	-1.258194	-1.184325
18	6	0	2.564938	-2.203048	2.679441
19	6	0	1.950159	-2.163680	1.281962
20	6	0	2.915407	-1.600680	0.238193
21	6	0	2.357695	-1.567260	-1.184325

22	1	0	1.318076	2.909543	3.413604
23	1	0	0.728448	4.409706	2.699736
24	1	0	-0.388917	3.082446	3.005020
25	1	0	0.822763	1.679982	1.307510
26	1	0	1.925349	2.992109	0.982248
27	1	0	0.000000	4.416366	0.215855
28	1	0	-1.098762	3.086645	0.520261
29	1	0	1.172111	3.098137	-1.525068
30	1	0	-0.561564	3.237753	-1.864944
31	1	0	-3.178777	-0.313284	3.413604
32	1	0	-4.183141	-1.573999	2.699736
33	1	0	-2.475018	-1.878035	3.005020
34	1	0	-1.866289	-0.127457	1.307510
35	1	0	-3.553917	0.171347	0.982248
36	1	0	-3.824685	-2.208183	0.215855
37	1	0	-2.123732	-2.494878	0.520261
38	1	0	-3.269120	-0.533991	-1.525068
39	1	0	-2.523195	-2.105205	-1.864944
40	1	0	1.860700	-2.596259	3.413604
41	1	0	3.454694	-2.835707	2.699736
42	1	0	2.863935	-1.204411	3.005020
43	1	0	1.043526	-1.552525	1.307510
44	1	0	1.628568	-3.163456	0.982248
45	1	0	3.824685	-2.208183	0.215855
46	1	0	3.222494	-0.591766	0.520261
47	1	0	2.097010	-2.564146	-1.525068
48	1	0	3.084759	-1.132548	-1.864944

Tri-*n*-butyl isocyanurate (C_s) (RB3LYP) = -978.300893292

1	7	0	-0.605857	-0.481105	1.175030
2	6	0	-0.878388	-1.169629	0.000000
3	7	0	-0.605857	-0.481105	-1.175030
4	6	0	0.006562	0.764372	-1.228407
5	7	0	0.316692	1.333668	-0.000000
6	6	0	0.006562	0.764372	1.228407
7	8	0	-1.339009	-2.291705	0.000000
8	8	0	0.260275	1.315440	-2.278800
9	8	0	0.260275	1.315440	2.278800
10	6	0	1.133679	-3.538188	4.771826
11	6	0	-0.034511	-2.693881	4.266079
12	6	0	0.274786	-1.995424	2.943129
13	6	0	-0.900120	-1.157195	2.451292
14	6	0	1.133679	-3.538188	-4.771826
15	6	0	-0.034511	-2.693881	-4.266079
16	6	0	0.274786	-1.995424	-2.943129
17	6	0	-0.900120	-1.157195	-2.451292
18	6	0	-0.415084	6.310599	-0.000000
19	6	0	0.597863	5.167250	-0.000000
20	6	0	-0.067979	3.792339	-0.000000
21	6	0	0.955411	2.662083	-0.000000
22	1	0	0.892531	-4.027628	5.716166
23	1	0	1.396055	-4.314978	4.050837
24	1	0	2.020967	-2.922486	4.932132
25	1	0	-0.297118	-1.943575	5.017675
26	1	0	-0.917907	-3.327156	4.142010
27	1	0	0.521068	-2.738844	2.181196
28	1	0	1.145747	-1.346430	3.062712
29	1	0	-1.145298	-0.381085	3.170921
30	1	0	-1.773254	-1.781845	2.284645
31	1	0	0.892531	-4.027628	-5.716166
32	1	0	2.020967	-2.922486	-4.932132
33	1	0	1.396055	-4.314978	-4.050837
34	1	0	-0.917907	-3.327156	-4.142010
35	1	0	-0.297118	-1.943575	-5.017675
36	1	0	1.145747	-1.346430	-3.062712
37	1	0	0.521068	-2.738844	-2.181196
38	1	0	-1.773254	-1.781845	-2.284645
39	1	0	-1.145298	-0.381085	-3.170921
40	1	0	0.080310	7.282232	-0.000000
41	1	0	-1.057989	6.263816	-0.881214
42	1	0	-1.057989	6.263816	0.881214
43	1	0	1.248089	5.253438	0.875566

44	1	0	1.248089	5.253438	-0.875566
45	1	0	-0.706160	3.690593	-0.881136
46	1	0	-0.706160	3.690593	0.881136
47	1	0	1.581672	2.712230	0.886342
48	1	0	1.581672	2.712230	-0.886342

Tri-*n*-hexyl isocyanurate (C_3) E(RB3LYP) = -1214.29375648

1	7	0	-0.677613	1.177286	-2.448513
2	6	0	0.711666	1.226158	-2.440486
3	7	0	1.358366	-0.001813	-2.448513
4	6	0	0.706051	-1.229400	-2.440486
5	7	0	-0.680753	-1.175473	-2.448513
6	6	0	-1.417717	0.003242	-2.440486
7	8	0	1.327796	2.270246	-2.412321
8	8	0	1.302193	-2.285028	-2.412321
9	8	0	-2.629988	0.014782	-2.412321
10	6	0	-1.419091	2.436570	-2.231421
11	6	0	-1.887925	2.580194	-0.780589
12	6	0	-0.774964	2.439165	0.258333
13	6	0	-1.283553	2.535962	1.695080
14	6	0	-0.187722	2.305625	2.735085
15	6	0	-0.708872	2.315816	4.170066
16	6	0	2.819677	0.010683	-2.231421
17	6	0	3.178476	0.344894	-0.780589
18	6	0	2.499861	-0.548444	0.258333
19	6	0	2.837984	-0.156391	1.695080
20	6	0	2.090591	-0.990240	2.735085
21	6	0	2.359992	-0.544007	4.170066
22	6	0	-1.400587	-2.447254	-2.231421
23	6	0	-1.290551	-2.925088	-0.780589
24	6	0	-1.724896	-1.890721	0.258333
25	6	0	-1.554431	-2.379571	1.695080
26	6	0	-1.902869	-1.315385	2.735085
27	6	0	-1.651120	-1.771809	4.170066
28	1	0	-0.742502	3.238176	-2.507760
29	1	0	-2.270599	2.435446	-2.906467
30	1	0	-2.361253	3.561098	-0.685742
31	1	0	-2.663772	1.837820	-0.588023
32	1	0	-0.285146	1.468098	0.136426
33	1	0	0.000000	3.189250	0.080865
34	1	0	-1.743209	3.515818	1.859634
35	1	0	-2.079662	1.799297	1.843495
36	1	0	0.297955	1.347544	2.533561
37	1	0	0.589460	3.066385	2.616718
38	1	0	0.093663	2.145790	4.889008
39	1	0	-1.177738	3.271614	4.412458
40	1	0	-1.456551	1.534030	4.317591
41	1	0	3.175594	-0.976062	-2.507760
42	1	0	3.244458	0.748673	-2.906467
43	1	0	4.264628	0.264356	-0.685742
44	1	0	2.923485	1.387984	-0.588023
45	1	0	1.413983	-0.487105	0.136426
46	1	0	2.761972	-1.594625	0.080865
47	1	0	3.916392	-0.248245	1.859634
48	1	0	2.598068	0.901391	1.843495
49	1	0	1.018030	-0.931809	2.533561
50	1	0	2.360837	-2.043680	2.616718
51	1	0	1.811478	-1.154009	4.889008
52	1	0	3.422170	-0.615856	4.412458
53	1	0	2.056785	0.494396	4.317591
54	1	0	-2.433092	-2.262114	-2.507760
55	1	0	-0.973859	-3.184119	-2.906467
56	1	0	-1.903375	-3.825454	-0.685742
57	1	0	-0.259713	-3.225805	-0.588023
58	1	0	-1.128837	-0.980993	0.136426
59	1	0	-2.761972	-1.594625	0.080865
60	1	0	-2.173183	-3.267572	1.859634
61	1	0	-0.518406	-2.700688	1.843495
62	1	0	-1.315985	-0.415736	2.533561
63	1	0	-2.950297	-1.022705	2.616718
64	1	0	-1.905140	-0.991781	4.889008
65	1	0	-2.244432	-2.655758	4.412458

66	1	0	-0.600233	-2.028426	4.317591

Tri-*n*-hexyl isocyanurate (C_s) E(RB3LYP) = -1214.28453811

1	7	0	-0.240161	1.402358	0.000000
2	6	0	0.119572	0.863022	1.228371
3	7	0	0.840874	-0.322717	1.175019
4	6	0	1.173700	-0.984149	-0.000000
5	7	0	0.840874	-0.322717	-1.175019
6	6	0	0.119572	0.863022	-1.228371
7	8	0	-0.182459	1.389185	2.278801
8	8	0	1.732575	-2.060719	-0.000000
9	8	0	-0.182459	1.389185	-2.278801
10	6	0	-0.994917	2.668523	0.000000
11	6	0	-0.076391	3.885527	0.000000
12	6	0	-0.863170	5.194406	0.000000
13	6	0	0.033537	6.431526	0.000000
14	6	0	-0.744805	7.746818	0.000000
15	6	0	0.161414	8.976647	0.000000
16	6	0	1.193533	-0.970394	2.451288
17	6	0	0.097824	-1.910542	2.941679
18	6	0	0.468462	-2.578864	4.263842
19	6	0	-0.613068	-3.527565	4.778436
20	6	0	-0.251396	-4.201791	6.101468
21	6	0	-1.339466	-5.147801	6.606322
22	6	0	1.193533	-0.970394	-2.451288
23	6	0	0.097824	-1.910542	-2.941679
24	6	0	0.468462	-2.578864	-4.263842
25	6	0	-0.613068	-3.527565	-4.778436
26	6	0	-0.251396	-4.201791	-6.101468
27	6	0	-1.339466	-5.147801	-6.606322
28	1	0	-1.623133	2.662584	-0.886323
29	1	0	-1.623133	2.662584	0.886323
30	1	0	0.568054	3.840435	0.881101
31	1	0	0.568054	3.840435	-0.881101
32	1	0	-1.519453	5.223654	-0.875926
33	1	0	-1.519453	5.223654	0.875926
34	1	0	0.691242	6.401006	0.874993
35	1	0	0.691242	6.401006	-0.874993
36	1	0	-1.401906	7.775443	-0.874468
37	1	0	-1.401906	7.775443	0.874468
38	1	0	-0.417380	9.901311	0.000000
39	1	0	0.806901	8.987983	0.880841
40	1	0	0.806901	8.987983	-0.880841
41	1	0	2.119116	-1.514400	2.285064
42	1	0	1.367796	-0.175832	3.171405
43	1	0	-0.827269	-1.341541	3.060749
44	1	0	-0.080248	-2.671838	2.178626
45	1	0	1.405594	-3.131616	4.141182
46	1	0	0.662894	-1.809229	5.017934
47	1	0	-1.550762	-2.975022	4.899088
48	1	0	-0.808822	-4.295905	4.023139
49	1	0	0.686011	-4.752846	5.979413
50	1	0	-0.055513	-3.432794	6.854833
51	1	0	-1.057605	-5.615695	7.550584
52	1	0	-2.279088	-4.614741	6.766387
53	1	0	-1.532170	-5.944419	5.884563
54	1	0	1.367796	-0.175832	-3.171405
55	1	0	2.119116	-1.514400	-2.285064
56	1	0	-0.080248	-2.671838	-2.178626
57	1	0	-0.827269	-1.341541	-3.060749
58	1	0	0.662894	-1.809229	-5.017934
59	1	0	1.405594	-3.131616	-4.141182
60	1	0	-0.808822	-4.295905	-4.023139
61	1	0	-1.550762	-2.975022	-4.899088
62	1	0	-0.055513	-3.432794	-6.854833
63	1	0	0.686011	-4.752846	-5.979413
64	1	0	-1.057605	-5.615695	-7.550584
65	1	0	-1.532170	-5.944419	-5.884563
66	1	0	-2.279088	-4.614741	-6.766387

Tri-*n*-octyl isocyanurate (C_3) E(RB3LYP) = -1450.28356961

1	7	0	0.063304	1.356432	3.578662

2	6	0	-1.194049	0.764067	3.569901
3	7	0	-1.206357	-0.623393	3.578662
4	6	0	-0.064677	-1.416111	3.569901
5	7	0	1.143053	-0.733039	3.578662
6	6	0	1.258726	0.652043	3.569901
7	8	0	-2.220199	1.409905	3.543363
8	8	0	-0.110914	-2.627701	3.543363
9	8	0	2.331113	1.217796	3.543363
10	6	0	0.146068	2.818183	3.384639
11	6	0	0.508672	3.186857	1.944054
12	6	0	-0.396582	2.560050	0.882816
13	6	0	0.000000	2.959226	-0.536644
14	6	0	-0.835780	2.278944	-1.619022
15	6	0	-0.441129	2.700520	-3.033416
16	6	0	-2.513652	-1.282592	3.384639
17	6	0	-3.014235	-1.152905	1.944054
18	6	0	-2.018777	-1.623475	0.882816
19	6	0	-2.562765	-1.479613	-0.536644
20	6	0	-1.555734	-1.863278	-1.619022
21	6	0	-2.118155	-1.732289	-3.033416
22	6	0	2.367584	-1.535590	3.384639
23	6	0	2.505563	-2.033952	1.944054
24	6	0	2.415359	-0.936575	0.882816
25	6	0	2.562765	-1.479613	-0.536644
26	6	0	2.391513	-0.415666	-1.619022
27	6	0	2.559284	-0.968231	-3.033416
28	1	0	-0.825637	3.214824	3.658819
29	1	0	0.896663	3.197525	4.072992
30	1	0	0.466659	4.276717	1.867280
31	1	0	1.544034	2.898957	1.756999
32	1	0	-0.349835	1.469218	0.961011
33	1	0	-1.438459	2.830679	1.072579
34	1	0	-0.079603	4.045776	-0.644732
35	1	0	1.055345	2.714910	-0.696399
36	1	0	-0.731884	1.193259	-1.523183
37	1	0	-1.896599	2.494326	-1.454749
38	1	0	-0.602704	3.777148	-3.150282
39	1	0	0.633414	2.541783	-3.167276
40	1	0	-2.371301	-2.322435	3.658819
41	1	0	-3.217469	-0.822230	4.072992
42	1	0	-3.937076	-1.734220	1.867280
43	1	0	-3.282587	-0.112306	1.756999
44	1	0	-1.097463	-1.037575	0.961011
45	1	0	-1.732211	-2.661082	1.072579
46	1	0	-3.463943	-2.091826	-0.644732
47	1	0	-2.878853	-0.443499	-0.696399
48	1	0	-0.667450	-1.230460	-1.523183
49	1	0	-1.211850	-2.889665	-1.454749
50	1	0	-2.969754	-2.410531	-3.150282
51	1	0	-2.517956	-0.722339	-3.167276
52	1	0	3.196938	-0.892390	3.658819
53	1	0	2.320807	-2.375295	4.072992
54	1	0	3.470416	-2.542498	1.867280
55	1	0	1.738554	-2.786651	1.756999
56	1	0	1.447297	-0.431643	0.961011
57	1	0	3.170670	-0.169597	1.072579
58	1	0	3.543546	-1.953950	-0.644732
59	1	0	1.823508	-2.271410	-0.696399
60	1	0	1.399334	0.037201	-1.523183
61	1	0	3.108449	0.395340	-1.454749
62	1	0	3.572458	-1.366617	-3.150282
63	1	0	1.884542	-1.819445	-3.167276
64	6	0	-1.197700	1.951239	-4.128454
65	1	0	-1.051938	0.878037	-3.989623
66	1	0	-2.271556	2.126074	-4.012446
67	6	0	-0.759277	2.341365	-5.538071
68	1	0	0.303187	2.137309	-5.685487
69	1	0	-1.311312	1.785519	-6.297292
70	1	0	-0.919397	3.405933	-5.720572
71	6	0	-1.090972	-2.012858	-4.128454
72	1	0	-0.234434	-1.350023	-3.989623
73	1	0	-0.705456	-3.030262	-4.012446

74	6	0	-1.648043	-1.828236	-5.538071
75	1	0	-2.002558	-0.806087	-5.685487
76	1	0	-0.890649	-2.028389	-6.297292
77	1	0	-2.489926	-2.499187	-5.720572
78	6	0	2.288672	0.061619	-4.128454
79	1	0	1.286371	0.471986	-3.989623
80	1	0	2.977012	0.904188	-4.012446
81	6	0	2.407320	-0.513129	-5.538071
82	1	0	2.201961	0.242869	-6.297292
83	1	0	3.409323	-0.906745	-5.720572
84	1	0	1.699370	-1.331223	-5.685487

Tri-*n*-octyl isocyanurate (C_s) E(RB3LYP) = -1450.26787905

1	7	0	1.055576	-0.165353	1.175021
2	6	0	1.419715	-0.810074	0.000000
3	7	0	1.055576	-0.165353	-1.175021
4	6	0	0.278256	0.984435	-1.228361
5	7	0	-0.106877	1.505934	0.000000
6	6	0	0.278256	0.984435	1.228361
7	8	0	2.029500	-1.858658	0.000000
8	8	0	-0.048705	1.495486	-2.278800
9	8	0	-0.048705	1.495486	2.278800
10	6	0	1.438225	-0.795777	2.451308
11	6	0	0.388215	-1.786980	2.941088
12	6	0	0.789514	-2.437388	4.263197
13	6	0	-0.246375	-3.436313	4.776998
14	6	0	0.147031	-4.092380	6.099602
15	6	0	-0.888122	-5.091332	6.614344
16	6	0	1.438225	-0.795777	-2.451308
17	6	0	0.388215	-1.786980	-2.941088
18	6	0	0.789514	-2.437388	-4.263197
19	6	0	-0.246375	-3.436313	-4.776998
20	6	0	0.147031	-4.092380	-6.099602
21	6	0	-0.888122	-5.091332	-6.614344
22	6	0	-0.921377	2.734531	0.000000
23	6	0	-0.062217	3.994127	0.000000
24	6	0	-0.910746	5.263810	0.000000
25	6	0	-0.074164	6.542496	0.000000
26	6	0	-0.915394	7.817963	0.000000
27	6	0	-0.080095	9.097294	0.000000
28	1	0	2.388662	-1.295158	2.285292
29	1	0	1.574304	0.006023	3.171629
30	1	0	-0.562879	-1.262527	3.059929
31	1	0	0.246711	-2.555654	2.177761
32	1	0	1.751746	-2.945222	4.140854
33	1	0	0.947070	-1.659702	5.017610
34	1	0	-1.208720	-2.928110	4.896918
35	1	0	-0.404959	-4.212164	4.020909
36	1	0	1.110117	-4.599554	5.979008
37	1	0	0.306616	-3.315617	6.854896
38	1	0	-1.851615	-4.584531	6.734926
39	1	0	-1.048299	-5.868279	5.859088
40	1	0	1.574304	0.006023	-3.171629
41	1	0	2.388662	-1.295158	-2.285292
42	1	0	0.246711	-2.555654	-2.177761
43	1	0	-0.562879	-1.262527	-3.059929
44	1	0	0.947070	-1.659702	-5.017610
45	1	0	1.751746	-2.945222	-4.140854
46	1	0	-0.404959	-4.212164	-4.020909
47	1	0	-1.208720	-2.928110	-4.896918
48	1	0	0.306616	-3.315617	-6.854896
49	1	0	1.110117	-4.599554	-5.979008
50	1	0	-1.048299	-5.868279	-5.859088
51	1	0	-1.851615	-4.584531	-6.734926
52	1	0	-1.548590	2.698510	-0.886322
53	1	0	-1.548590	2.698510	0.886322
54	1	0	0.583664	3.979965	0.881098
55	1	0	0.583664	3.979965	-0.881098
56	1	0	-1.567697	5.261661	-0.875889
57	1	0	-1.567697	5.261661	0.875889
58	1	0	0.584012	6.542686	0.874957
59	1	0	0.584012	6.542686	-0.874957

60	1	0	-1.574166	7.816349	-0.874829
61	1	0	-1.574166	7.816349	0.874829
62	1	0	0.579144	9.099257	0.874701
63	1	0	0.579144	9.099257	-0.874701
64	6	0	-0.496833	-5.749124	7.937371
65	1	0	0.465592	-6.255490	7.815920
66	1	0	-0.337310	-4.972292	8.691360
67	6	0	-1.539347	-6.745479	8.441673
68	1	0	-1.694323	-7.549952	7.719471
69	1	0	-1.236507	-7.200215	9.385962
70	1	0	-2.503151	-6.257274	8.601372
71	6	0	-0.496833	-5.749124	-7.937371
72	1	0	-0.337310	-4.972292	-8.691360
73	1	0	0.465592	-6.255490	-7.815920
74	6	0	-1.539347	-6.745479	-8.441673
75	1	0	-2.503151	-6.257274	-8.601372
76	1	0	-1.236507	-7.200215	-9.385962
77	1	0	-1.694323	-7.549952	-7.719471
78	6	0	-0.919492	10.374637	0.000000
79	1	0	-1.577520	10.372002	-0.874308
80	1	0	-1.577520	10.372002	0.874308
81	6	0	-0.073466	11.646692	0.000000
82	1	0	-0.695639	12.542840	0.000000
83	1	0	0.570928	11.688916	0.880761
84	1	0	0.570928	11.688916	-0.880761

Tri-*i*-propyl isocyanurate (C_{3h}) E(RB3LYP) = -860.305801320

1	7	0	1.344802	-0.226346	0.000000
2	6	0	0.489763	-1.330156	0.000000
3	7	0	-0.868422	-1.051459	0.000000
4	6	0	-1.396830	0.240930	0.000000
5	7	0	-0.476379	1.277805	0.000000
6	6	0	0.907067	1.089225	0.000000
7	8	0	0.910495	-2.468478	0.000000
8	8	0	-2.593013	0.445727	0.000000
9	8	0	1.682517	2.022751	0.000000
10	6	0	2.815791	-0.503784	0.000000
11	6	0	3.482838	0.000000	1.277850
12	6	0	3.482838	0.000000	-1.277850
13	6	0	-1.844185	-2.186655	0.000000
14	6	0	-1.741419	-3.016226	1.277850
15	6	0	-1.741419	-3.016226	-1.277850
16	6	0	-0.971606	2.690439	0.000000
17	6	0	-1.741419	3.016226	1.277850
18	6	0	-1.741419	3.016226	-1.277850
19	1	0	2.860086	-1.587257	0.000000
20	1	0	2.975395	-0.395598	2.158383
21	1	0	4.514793	-0.351899	1.300218
22	1	0	3.484819	1.085446	1.328181
23	1	0	2.975395	-0.395598	-2.158383
24	1	0	4.514793	-0.351899	-1.300218
25	1	0	3.484819	1.085446	-1.328181
26	1	0	-2.804648	-1.683279	0.000000
27	1	0	-1.830295	-2.378969	2.158383
28	1	0	-2.562150	-3.733976	1.300218
29	1	0	-0.802385	-3.560665	1.328181
30	1	0	-1.830295	-2.378969	-2.158383
31	1	0	-2.562150	-3.733976	-1.300218
32	1	0	-0.802385	-3.560665	-1.328181
33	1	0	-0.055438	3.270536	0.000000
34	1	0	-1.145100	2.774567	2.158383
35	1	0	-1.952643	4.085875	1.300218
36	1	0	-2.682433	2.475218	1.328181
37	1	0	-1.145100	2.774567	-2.158383
38	1	0	-1.952643	4.085875	-1.300218
39	1	0	-2.682433	2.475218	-1.328181

Tri-*i*-propyl isocyanurate (C_s) E(RB3LYP) = -860.305695683

1	7	0	1.491644	-0.071281	0.000000
2	6	0	0.837782	1.152811	0.000000
3	7	0	-0.556284	1.105571	0.000000
4	6	0	-1.288247	-0.074240	0.000000

5	7	0	-0.554562	-1.254585	0.000000
6	6	0	0.837480	-1.302461	0.000000
7	8	0	1.446248	2.202838	0.000000
8	8	0	-2.501810	-0.075581	0.000000
9	8	0	1.445444	-2.352741	0.000000
10	6	0	2.989241	-0.094227	0.000000
11	6	0	3.560857	0.515658	1.277852
12	6	0	3.560857	0.515658	-1.277852
13	6	0	-1.283804	2.413300	0.000000
14	6	0	-2.097988	2.603944	1.277766
15	6	0	-2.097988	2.603944	-1.277766
16	6	0	-1.283689	-2.562398	0.000000
17	6	0	-2.097988	-2.752414	-1.277774
18	6	0	-2.097988	-2.752414	1.277774
19	1	0	3.217520	-1.154165	0.000000
20	1	0	3.127613	0.040049	2.158433
21	1	0	4.637443	0.343255	1.300383
22	1	0	3.379321	1.585788	1.327940
23	1	0	3.127613	0.040049	-2.158433
24	1	0	4.637443	0.343255	-1.300383
25	1	0	3.379321	1.585788	-1.327940
26	1	0	-0.479463	3.140614	0.000000
27	1	0	-1.470054	2.464712	2.158458
28	1	0	-2.485873	3.622907	1.301130
29	1	0	-2.934675	1.912413	1.326830
30	1	0	-1.470054	2.464712	-2.158458
31	1	0	-2.485873	3.622907	-1.301130
32	1	0	-2.934675	1.912413	-1.326830
33	1	0	-0.480248	-3.290505	0.000000
34	1	0	-1.470164	-2.612974	-2.158508
35	1	0	-2.485561	-3.771493	-1.301307
36	1	0	-2.934848	-2.061143	-1.326601
37	1	0	-1.470164	-2.612974	2.158508
38	1	0	-2.485561	-3.771493	1.301307
39	1	0	-2.934848	-2.061143	1.326601

Tri-*t*-butyl isocyanurate(C_s) E(RB3LYP) = -978.263023744

1	7	0	0.029129	-0.657451	1.171900
2	6	0	0.619624	-1.167042	0.000000
3	7	0	0.029129	-0.657451	-1.171900
4	6	0	-0.248519	0.704342	-1.209139
5	7	0	-0.011235	1.376847	0.000000
6	6	0	-0.248519	0.704342	1.209139
7	8	0	1.507817	-1.979980	0.000000
8	8	0	-0.621831	1.276945	-2.210703
9	8	0	-0.621831	1.276945	2.210703
10	6	0	-0.114117	-1.504067	2.429058
11	6	0	0.954269	-1.082638	3.441313
12	6	0	0.034969	-2.997250	2.101741
13	6	0	-1.535945	-1.313835	2.989507
14	6	0	-0.114117	-1.504067	-2.429058
15	6	0	0.034969	-2.997250	-2.101741
16	6	0	0.954269	-1.082638	-3.441313
17	6	0	-1.535945	-1.313835	-2.989507
18	6	0	0.170380	2.889008	0.000000
19	6	0	-1.201641	3.565089	0.000000
20	6	0	0.996058	3.308539	-1.230665
21	6	0	0.996058	3.308539	1.230665
22	1	0	0.839838	-0.036347	3.713799
23	1	0	0.862396	-1.687041	4.344459
24	1	0	1.948988	-1.239113	3.024363
25	1	0	-0.638320	-3.298393	1.298416
26	1	0	-0.244190	-3.555888	2.994108
27	1	0	1.045904	-3.270031	1.823992
28	1	0	-1.665922	-1.989538	3.834664
29	1	0	-1.717046	-0.300461	3.324455
30	1	0	-2.277850	-1.573951	2.233225
31	1	0	-0.638320	-3.298393	-1.298416
32	1	0	-0.244190	-3.555888	-2.994108
33	1	0	1.045904	-3.270031	-1.823992
34	1	0	0.839838	-0.036347	-3.713799
35	1	0	0.862396	-1.687041	-4.344459

36	1	0	1.948988	-1.239113	-3.024363
37	1	0	-1.665922	-1.989538	-3.834664
38	1	0	-2.277850	-1.573951	-2.233225
39	1	0	-1.717046	-0.300461	-3.324455
40	1	0	-1.761944	3.279451	0.888511
41	1	0	-1.080254	4.649162	0.000000
42	1	0	-1.761944	3.279451	-0.888511
43	1	0	1.912732	2.720382	-1.298203
44	1	0	1.279131	4.352637	-1.104406
45	1	0	0.449842	3.209555	-2.159589
46	1	0	1.279131	4.352637	1.104406
47	1	0	0.449842	3.209555	2.159589
48	1	0	1.912732	2.720382	1.298203

Tri-*t*-butyl isocyanurate(C_{3v}) E(RB3LYP) = -978.261636690

1	7	0	0.000000	1.367030	-0.013250
2	6	0	-1.204820	0.695603	0.227657
3	7	0	-1.183882	-0.683515	-0.013250
4	6	0	-0.000000	-1.391206	0.227657
5	7	0	1.183882	-0.683515	-0.013250
6	6	0	1.204820	0.695603	0.227657
7	8	0	-2.192745	1.265982	0.632393
8	8	0	-0.000000	-2.531964	0.632393
9	8	0	2.192745	1.265982	0.632393
10	6	0	0.000000	2.888752	-0.123609
11	6	0	1.230247	3.340566	-0.933213
12	6	0	-1.230247	3.340566	-0.933213
13	6	0	0.000000	3.509133	1.274394
14	6	0	-2.501733	-1.444376	-0.123609
15	6	0	-3.508138	-0.604857	-0.933213
16	6	0	-2.277891	-2.735708	-0.933213
17	6	0	-3.038998	-1.754567	1.274394
18	6	0	2.501733	-1.444376	-0.123609
19	6	0	3.038998	-1.754567	1.274394
20	6	0	2.277891	-2.735708	-0.933213
21	6	0	3.508138	-0.604857	-0.933213
22	1	0	2.159623	3.222890	-0.391797
23	1	0	1.102471	4.394334	-1.176723
24	1	0	1.297747	2.787497	-1.871438
25	1	0	-2.159623	3.222890	-0.391797
26	1	0	-1.102471	4.394334	-1.176723
27	1	0	-1.297747	2.787497	-1.871438
28	1	0	0.000000	4.596981	1.194202
29	1	0	0.888486	3.203353	1.823615
30	1	0	-0.888486	3.203353	1.823615
31	1	0	-3.870917	0.258843	-0.391797
32	1	0	-4.356840	-1.242399	-1.176723
33	1	0	-3.062917	-0.269866	-1.871438
34	1	0	-1.711293	-3.481734	-0.391797
35	1	0	-3.254369	-3.151935	-1.176723
36	1	0	-1.765169	-2.517631	-1.871438
37	1	0	-3.981102	-2.298491	1.194202
38	1	0	-3.218428	-0.832225	1.823615
39	1	0	-2.329942	-2.371128	1.823615
40	1	0	3.218428	-0.832225	1.823615
41	1	0	3.981102	-2.298491	1.194202
42	1	0	2.329942	-2.371128	1.823615
43	1	0	1.765169	-2.517631	-1.871438
44	1	0	3.254369	-3.151935	-1.176723
45	1	0	1.711293	-3.481734	-0.391797
46	1	0	4.356840	-1.242399	-1.176723
47	1	0	3.870917	0.258843	-0.391797
48	1	0	3.062917	-0.269866	-1.871438

Tricyclohexyl isocyanurate(C_{3h}) E(RB3LYP) = -1210.65474074

1	7	0	-0.956564	-0.972888	0.000000
2	6	0	0.384128	-1.364649	0.000000
3	7	0	1.320827	-0.341965	0.000000
4	6	0	0.989756	1.014989	0.000000
5	7	0	-0.364263	1.314852	0.000000
6	6	0	-1.373885	0.349659	0.000000
7	8	0	0.709920	-2.533697	0.000000

8	8	0	1.839286	1.881657	0.000000
9	8	0	-2.549206	0.652040	0.000000
10	6	0	-1.978622	-2.060232	0.000000
11	6	0	-2.828590	-2.064753	1.273987
12	6	0	-2.828590	-2.064753	-1.273987
13	1	0	-1.380768	-2.966933	0.000000
14	6	0	-3.774947	-3.270642	1.263497
15	1	0	-3.405848	-1.143565	1.335438
16	1	0	-2.171355	-2.103427	2.145525
17	6	0	-3.774947	-3.270642	-1.263497
18	1	0	-3.405848	-1.143565	-1.335438
19	1	0	-2.171355	-2.103427	-2.145525
20	6	0	-4.640523	-3.289808	0.000000
21	1	0	-4.403120	-3.251656	2.155995
22	1	0	-3.189296	-4.194608	1.312053
23	1	0	-4.403120	-3.251656	-2.155995
24	1	0	-3.189296	-4.194608	-1.312053
25	1	0	-5.288658	-4.168611	0.000000
26	1	0	-5.295997	-2.413193	0.000000
27	6	0	2.773525	-0.683421	0.000000
28	6	0	3.202424	-1.417255	1.273987
29	6	0	3.202424	-1.417255	-1.273987
30	1	0	3.259823	0.287686	0.000000
31	6	0	4.719932	-1.633879	1.263497
32	1	0	2.693280	-2.377769	1.335438
33	1	0	2.907298	-0.828735	2.145525
34	6	0	4.719932	-1.633879	-1.263497
35	1	0	2.693280	-2.377769	-1.335438
36	1	0	2.907298	-0.828735	-2.145525
37	6	0	5.169319	-2.373907	0.000000
38	1	0	5.017577	-2.187386	2.155995
39	1	0	5.227285	-0.664707	1.312053
40	1	0	5.017577	-2.187386	-2.155995
41	1	0	5.227285	-0.664707	-1.312053
42	1	0	6.254452	-2.495806	0.000000
43	1	0	4.737885	-3.379871	0.000000
44	6	0	-0.794903	2.743653	0.000000
45	6	0	-0.373833	3.482007	1.273987
46	6	0	-0.373833	3.482007	-1.273987
47	1	0	-1.879055	2.679247	0.000000
48	6	0	-0.944985	4.904521	1.263497
49	1	0	0.712568	3.521334	1.335438
50	1	0	-0.735944	2.932162	2.145525
51	6	0	-0.944985	4.904521	-1.263497
52	1	0	0.712568	3.521334	-1.335438
53	1	0	-0.735944	2.932162	-2.145525
54	6	0	-0.528795	5.663715	0.000000
55	1	0	-0.614456	5.439042	2.155995
56	1	0	-2.037989	4.859315	1.312053
57	1	0	-0.614456	5.439042	-2.155995
58	1	0	-2.037989	4.859315	-1.312053
59	1	0	-0.965794	6.664417	0.000000
60	1	0	0.558112	5.793065	0.000000

Triphenyl isocyanurate(D_3) E(RB3LYP) = -1199.71512245

1	7	0	0.000000	1.359872	0.000000
2	6	0	1.239791	0.715794	0.000000
3	7	0	1.177684	-0.679936	0.000000
4	6	0	0.000000	-1.431587	0.000000
5	7	0	-1.177684	-0.679936	0.000000
6	6	0	-1.239791	0.715794	0.000000
7	8	0	2.283282	1.318253	0.000000
8	8	0	0.000000	-2.636507	0.000000
9	8	0	-2.283282	1.318253	0.000000
10	6	0	0.000000	2.804957	0.000000
11	6	0	2.429164	-1.402478	0.000000
12	6	0	-2.429164	-1.402478	0.000000
13	6	0	0.341112	3.487589	1.157293
14	6	0	0.343625	4.876159	1.154248
15	6	0	0.000000	5.571084	0.000000
16	6	0	-0.343625	4.876159	-1.154248
17	6	0	-0.341112	3.487589	-1.157293

18	6	0	-3.190897	-1.448382	1.157293
19	6	0	-4.394690	-2.140491	1.154248
20	6	0	-4.824700	-2.785542	0.000000
21	6	0	-4.051065	-2.735667	-1.154248
22	6	0	-2.849784	-2.039206	-1.157293
23	6	0	2.849784	-2.039206	1.157293
24	6	0	4.051065	-2.735667	1.154248
25	6	0	4.824700	-2.785542	0.000000
26	6	0	4.394690	-2.140491	-1.154248
27	6	0	3.190897	-1.448382	-1.157293
28	1	0	0.612153	2.934268	2.045115
29	1	0	0.613554	5.413701	2.052840
30	1	0	0.000000	6.652638	0.000000
31	1	0	-0.613554	5.413701	-2.052840
32	1	0	-0.612153	2.934268	-2.045115
33	1	0	-2.847227	-0.936994	2.045115
34	1	0	-4.995179	-2.175497	2.052840
35	1	0	-5.761353	-3.326319	0.000000
36	1	0	-4.381625	-3.238204	-2.052840
37	1	0	-2.235075	-1.997274	-2.045115
38	1	0	2.235075	-1.997274	2.045115
39	1	0	4.381625	-3.238204	2.052840
40	1	0	5.761353	-3.326319	0.000000
41	1	0	4.995179	-2.175497	-2.052840
42	1	0	2.847227	-0.936994	-2.045115

The Cartesian coordinates of the optimized isocyanate

Methyl isocyanate (C_s) **E(RB3LYP) = -208.073147882**

1	6	0	1.340406	1.106070	0.000000
2	1	0	1.294021	2.192579	0.000000
3	1	0	1.886834	0.783661	0.887527
4	1	0	1.886834	0.783661	-0.887527
5	7	0	0.000000	0.579737	0.000000
6	6	0	-0.559972	-0.478178	0.000000
7	8	0	-1.218786	-1.448176	0.000000

Ethyl isocyanate (C_s) **E(RB3LYP) = -247.406675331**

1	7	0	0.000000	0.285177	0.000000
2	6	0	1.036884	0.884473	0.000000
3	8	0	1.983858	1.575969	0.000000
4	6	0	-1.993988	-1.129384	0.000000
5	6	0	-0.473346	-1.085150	0.000000
6	1	0	-2.338273	-2.164083	0.000000
7	1	0	-2.393856	-0.631382	0.882955
8	1	0	-2.393856	-0.631382	-0.882955
9	1	0	-0.081091	-1.598387	-0.880924
10	1	0	-0.081091	-1.598387	0.880924

***n*-Propyl isocyanate(C_1)** **E(RB3LYP) = -286.738234379**

1	7	0	0.671129	-0.861808	-0.181283
2	6	0	1.546077	-0.056366	-0.042750
3	8	0	2.471594	0.662654	0.011753
4	6	0	-1.514240	1.289842	0.122337
5	6	0	-1.708662	-0.164066	-0.299775
6	6	0	-0.672009	-1.119652	0.293956
7	1	0	-2.295294	1.925115	-0.295613
8	1	0	-1.547516	1.391298	1.209257
9	1	0	-0.556586	1.683129	-0.220651
10	1	0	-1.680631	-0.248291	-1.388271
11	1	0	-2.693591	-0.515276	0.019284
12	1	0	-0.917628	-2.145448	0.022666
13	1	0	-0.686402	-1.057651	1.385691

***n*-Butyl isaocyanate (C_1)** **E(RB3LYP) = -326.068771858**

1	7	0	1.441461	0.712698	-0.247474
2	6	0	1.963502	-0.349358	-0.066737
3	8	0	2.559335	-1.356259	0.022001
4	6	0	-2.745294	-0.942492	-0.128125
5	6	0	-1.376758	-0.444848	0.334087
6	6	0	-1.032484	0.932404	-0.230205
7	6	0	0.315023	1.482214	0.238690
8	1	0	-2.970730	-1.926140	0.284851
9	1	0	-3.538568	-0.259755	0.183260
10	1	0	-2.785551	-1.021167	-1.216350
11	1	0	-0.612870	-1.167012	0.036430
12	1	0	-1.350046	-0.401891	1.427363
13	1	0	-1.801445	1.651322	0.068717
14	1	0	-1.040473	0.899729	-1.322789
15	1	0	0.347450	1.517034	1.331162
16	1	0	0.443392	2.501549	-0.122595

***n*-hexyl isocyanate (C_1)** **E(RB3LYP) = -404.730027282**

1	7	0	2.683294	-0.256377	-0.222780
2	6	0	2.695779	0.932969	-0.087395
3	8	0	2.803465	2.100433	-0.038491
4	6	0	1.963584	-1.412728	0.269291
5	6	0	0.520250	-1.478996	-0.231358
6	6	0	-0.373731	-0.356271	0.290591
7	6	0	-1.818108	-0.466617	-0.196504
8	6	0	-2.718948	0.655931	0.317693
9	6	0	-4.159765	0.538004	-0.175838
10	1	0	2.510130	-2.294667	-0.061616
11	1	0	1.982652	-1.408850	1.362629
12	1	0	0.525120	-1.474837	-1.324298
13	1	0	0.111184	-2.445532	0.077935
14	1	0	-0.358127	-0.361606	1.385796
15	1	0	0.029398	0.612622	-0.016479

16	1	0	-1.830532	-0.466346	-1.291506
17	1	0	-2.232972	-1.432560	0.110780
18	1	0	-2.704654	0.655545	1.411795
19	1	0	-2.302844	1.619569	0.009436
20	1	0	-4.780988	1.349786	0.204753
21	1	0	-4.204337	0.568267	-1.266560
22	1	0	-4.609165	-0.403967	0.145850

***n*-Octyl isocyanate (C_1)** **E(RB3LYP) = -483.391146175**

1	7	0	-3.831270	0.032973	-0.221490
2	6	0	-3.651884	1.211350	-0.110856
3	8	0	-3.570933	2.381742	-0.085569
4	6	0	-3.300690	-1.214088	0.289004
5	6	0	-1.888631	-1.516360	-0.213945
6	6	0	-0.825507	-0.540854	0.286269
7	6	0	0.580669	-0.886490	-0.202857
8	6	0	1.649311	0.087935	0.290252
9	6	0	3.055670	-0.253591	-0.199466
10	6	0	4.126195	0.719899	0.292999
11	6	0	5.527708	0.368932	-0.203342
12	1	0	-3.313155	-1.188490	1.382151
13	1	0	-3.981619	-2.003964	-0.024777
14	1	0	-1.636087	-2.530175	0.111032
15	1	0	-1.898429	-1.529794	-1.306787
16	1	0	-1.071765	0.474471	-0.036203
17	1	0	-0.835844	-0.525552	1.381425
18	1	0	0.838290	-1.900777	0.119722
19	1	0	0.586273	-0.906069	-1.297575
20	1	0	1.389795	1.101540	-0.032272
21	1	0	1.642532	0.108088	1.385161
22	1	0	3.315353	-1.267915	0.122355
23	1	0	3.062829	-0.273254	-1.294557
24	1	0	3.865993	1.732690	-0.029089
25	1	0	4.118658	0.738741	1.387066
26	1	0	6.272001	1.078030	0.161709
27	1	0	5.824525	-0.627222	0.131900
28	1	0	5.569966	0.374516	-1.294627

***i*-Propyl isocyanate (C_s)** **E(RB3LYP) = -286.741493078**

1	7	0	0.063332	0.852756	0.000000
2	6	0	1.260943	0.798739	-0.000000
3	8	0	2.431599	0.873873	-0.000000
4	6	0	-1.062717	-0.070677	0.000000
5	6	0	-1.062717	-0.921666	1.269212
6	6	0	-1.062717	-0.921666	-1.269212
7	1	0	-1.956318	0.554975	0.000000
8	1	0	-1.056667	-0.292338	2.158217
9	1	0	-1.950412	-1.554697	1.297975
10	1	0	-0.181195	-1.564781	1.295629
11	1	0	-1.056667	-0.292338	-2.158217
12	1	0	-1.950412	-1.554697	-1.297975
13	1	0	-0.181195	-1.564781	-1.295629

Cyclohexyl isocyanate (C_s) **E(RB3LYP) = -403.524684021**

1	6	0	-0.705747	0.198213	0.000000
2	6	0	-0.034948	-0.351658	1.264143
3	6	0	-0.034948	-1.883275	1.263692
4	6	0	0.624548	-2.443389	0.000000
5	6	0	-0.034948	-1.883275	-1.263692
6	6	0	-0.034948	-0.351658	-1.264143
7	7	0	-0.728373	1.649818	0.000000
8	6	0	0.059874	2.553027	0.000000
9	8	0	0.730039	3.516124	0.000000
10	1	0	-1.750770	-0.120570	0.000000
11	1	0	0.994504	0.019135	1.296473
12	1	0	-0.544275	0.039267	2.146051
13	1	0	0.473495	-2.252261	2.156199
14	1	0	-1.067114	-2.243757	1.322490
15	1	0	1.686185	-2.175838	0.000000
16	1	0	0.576372	-3.533995	0.000000
17	1	0	0.473495	-2.252261	-2.156199
18	1	0	-1.067114	-2.243757	-1.322490

19	1	0	0.994504	0.019135	-1.296473
20	1	0	-0.544275	0.039267	-2.146051

_t_-Butyl isocyanate (C_s) E(RB3LYP) = -326.075222093

1	7	0	0.781572	0.322357	0.000000
2	6	0	1.687649	-0.462642	0.000000
3	8	0	2.649871	-1.133758	0.000000
4	6	0	-0.685370	0.290384	0.000000
5	6	0	-1.169780	1.742403	0.000000
6	6	0	-1.169780	-0.435231	1.261053
7	6	0	-1.169780	-0.435231	-1.261053
8	1	0	-0.806422	2.267037	-0.883225
9	1	0	-2.259491	1.775048	0.000000
10	1	0	-0.806422	2.267037	0.883225
11	1	0	-0.820889	-1.468446	1.269449
12	1	0	-2.259810	-0.440523	1.296565
13	1	0	-0.796936	0.062145	2.155965
14	1	0	-2.259810	-0.440523	-1.296565
15	1	0	-0.796936	0.062145	-2.155965
16	1	0	-0.820889	-1.468446	-1.269449

Phenyl isocyanate (C_s) E(RB3LYP) = -399.886593579

1	7	0	1.161964	1.053305	0.000000
2	6	0	2.355501	0.917221	0.000000
3	8	0	3.524715	0.910678	0.000000
4	6	0	-0.000000	0.278822	-0.000000
5	6	0	-1.231246	0.932076	-0.000000
6	6	0	-2.405541	0.191559	-0.000000
7	6	0	-2.362263	-1.198029	-0.000000
8	6	0	-1.131605	-1.846975	0.000000
9	6	0	0.048314	-1.117462	0.000000
10	1	0	-1.252470	2.012460	-0.000000
11	1	0	-3.357746	0.704523	-0.000000
12	1	0	-3.278849	-1.771467	-0.000000
13	1	0	-1.087880	-2.927786	0.000000
14	1	0	1.006513	-1.619563	0.000000