Electronic Supplementary Material (ESI)

for

Urea Hydrogen-Bond Donor Strengths: Bigger is not Always Better

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Method S1. Computational details

All calculations were performed using the Amsterdam Density Functional (ADF) program as implemented in the Amsterdam Modeling Suite (AMS, version 2023.1).[S1] The dispersion-corrected relativistic density functional theory (DFT-D) calculations were performed at the ZORA-BLYP-D3(BJ)[S2]/TZ2P level of theory, which has been proven to be adequate for studying these types of hydrogen-bonded systems.[S3] The TZ2P basis set[S1a,b] consists of an uncontracted set of Slater-type orbitals (STOs) of triple-ζ quality for all atoms, augmented with two sets of polarization functions. The ZlmFit[S4a] density fitting scheme with the Becke[S4b,c] integration grid, at "Excellent" quality, was used for geometry optimizations and subsequent (bonding) analyses. All optimized geometries have been checked to be energy minima by performing a vibrational frequency analysis (*i.e.,* no imaginary frequencies for minima, see Data S6 and S7).[S5] The ball-and-stick structures of the optimized structures in this work were created using the CYLview20[S6] visualization software.

[S1] (a) G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen and J. G. Snijders, T. Ziegler, *J. Comput. Chem*., 2001, **22**, 931; (b) E. van Lenthe, E. J. Baerends, *J. Comput. Chem.,* 2003, **24**, 1142; (c) C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Acc*., 1998, **99**, 391; (d) ADF 2023.1, SCM, Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands, www.scm.com; (e) AMS 2023.1, SCM, Theoretical Chemistry, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands, www.scm.com.

[S2] (a) E. van Lenthe, A. Ehlers and E. J. Baerends, *J. Chem. Phys.,* 1999, **110**, 8943; (b) A. D. Becke, *Phys. Rev. A,* 1988, **38**, 3098; (c) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785; (d) Q. Wu and W. Yang, *J. Chem. Phys*., 2002, **116**, 515; (e) S. Grimme, *J. Comput. Chem.,* 2004, **25**, 1463; (f) S. Grimme, *J. Comput. Chem.,* 2006, **27**, 1787; (g) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.,* 2010, **132**, 154104; (h) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.,* 2011, **32**, 1456; (i) A. D. Becke and E. R. Johnson, *J. Chem. Phys.,* 2005, **122**, 154101; (j) E. R. Johnson and A. D. Becke, *J. Chem. Phys.,* 2006, **124**, 024101.

[S3] C. Nieuwland and C. Fonseca Guerra, *Chem. Eur. J.,* 2022, **28**, e202200755.

[S4] (a) M. Franchini, P. H. T. Philipsen, E. van Lenthe and L. Visscher, *J. Chem. Theory Comput.,* 2014, **10**, 1994; (b) A. D. Becke, *J. Chem. Phys.,* 1998, **88**, 2547; (c) M. Franchini, P. H. T. Philipsen and L. Visscher, *J. Comput. Chem.,* 2013, **34**, 1819.

[S5] (a) S. K. Wolff, *Int. J. Quantum Chem.,* 2005, **104**, 645; (b) A. Bérces, R. M. Dickson, L. Fan, H. Jacobsen, D. P. Swerhone and T. Ziegler, *Comput. Phys. Commun.,* 1997, **100**, 247; (c) H. Jacobsen, A. Bérces, D. P. Swerhone and T. Ziegler, *Comput. Phys. Commun.,* 1997, **100**, 263.

[S6] C. Y. Legault, *CYLview20*, Université de Sherbrooke, Sherbrooke, Quebec, Canada, 2020, www.cylview.org.

Method S2. Hydrogen-bond and interaction energy analyses

In this work, the hydrogen-bond energy between the various urea hydrogen-bond donors (**X-urea**, with X = O, S, Se, C, Si, or Ge) and the hydrogen-bond acceptor formaldehyde (**F**) was computed. The hydrogen-bond energy (ΔE) is computed following Equation S1.

$$\Delta E = E(\mathbf{F}\cdots\mathbf{X\text{-}urea}) - E(\mathbf{F}) - E(\mathbf{X\text{-}urea}) \quad \text{(S1)}$$

In this equation, E(**F**$\cdots$**X-urea**), E(**F**), and E(**X-urea**) correspond to the electronic energies E of the formaldehyde–X-urea hydrogen-bonded complex (**F**$\cdots$**X-urea**), formaldehyde, and the X-urea, each in their optimized geometry, respectively.

To understand the different components that determine the relative stabilities of the **F**$\cdots$**X-urea** complexes, ΔE was partitioned according to the activation strain model (ASM)[S7] of reactivity and bonding into a strain and interaction energy component (Equation S2).

$$\Delta E = \Delta E_{\text{strain}} + \Delta E_{\text{int}} \quad \text{(S2)}$$

In this decomposition, the strain energy (ΔE_{strain}) is the energy required to deform the separately optimized geometries of the X-urea and formaldehyde molecules, to the geometry they acquire in the hydrogen-bonded complex. The interaction energy (ΔE_{int}) accounts for the stabilizing interaction between the two prepared (*i.e.,* deformed) molecules.

The interaction energy ΔE_{int} can be further decomposed based on Kohn-Sham molecular orbital theory using a quantitative energy decomposition analysis (EDA).[S8] In the EDA, the total interaction energy (ΔE_{int}) is decomposed into components of electrostatic interaction (ΔV_{elstat}), Pauli repulsion (ΔE_{Pauli}), orbital interaction (ΔE_{oi}), and dispersion (ΔE_{disp}) (see Equation S3).

$$\Delta E_{\text{int}} = \Delta V_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} \quad \text{(S3)}$$

[S7] (a) P. Vermeeren, S. C. C. van der Lubbe, C. Fonseca Guerra, F. M. Bickelhaupt and T. A. Hamlin, *Nat. Protoc.,* 2020, **15**, 649; (b) P. Vermeeren, T. A. Hamlin and F. M. Bickelhaupt, *Chem. Commun.,* 2021, **57**, 5880.

[S8] (a) F. M. Bickelhaupt and E. J. Baerends, in *Reviews in Computational Chemistry*, eds. K. B. Lipkowitz and D. B. Boyd, Wiley-VCH, New York, Vol. **15**, 2000, pp. 1–86; (b) T. A. Hamlin, P. Vermeeren, C. Fonseca Guerra and F. M. Bickelhaupt, in *Complementary Bonding Analysis*, ed. S. Grabowsky, De Gruyter, Berlin, 2021, pp. 199–212.

Here, ΔV_{elstat} comprises the (usually attractive) classical electrostatic interactions between the unperturbed charge distributions of the prepared (*i.e.,* deformed) interacting molecules, that is, the X-urea and formaldehyde. ΔE_{Pauli} accounts for the destabilizing interactions between the interacting molecules resulting from overlapping closed-shell orbitals and accounts for any steric repulsion. The ΔE_{oi} term comprises charge transfer between the interacting molecules (*i.e.,* donor–acceptor interactions between occupied and unoccupied orbitals on the interacting molecules, including HOMO–LUMO interactions) and mutual polarization of the interacting molecules (*i.e.,* empty–occupied orbital mixing on one molecule due to the presence of the other molecule).

Method S3. Voronoi deformation density (VDD) charges

The Voronoi deformation density (VDD) charge analysis allows for the quantification of the flow of electronic charge as a direct consequence of chemical-bond formation.[S9] VDD atomic charges (Q) are computed by the spatial integration of the deformation density over the Voronoi cell of atom A, which is the space defined by the bond midplanes on and perpendicular to all bond axes between this atom A and its neighboring atoms (see Equation S4).

$$Q = -\int_{\text{Voronoi cell of A}} [\rho(\mathbf{r}) - \sum_i \rho_i(\mathbf{r})]d\mathbf{r} \qquad \text{(S4)}$$

Herein, the deformation density $\Delta\rho(\mathbf{r}) = [\rho(\mathbf{r}) - \sum_i \rho_i(\mathbf{r})]$ is the density change going from a superposition of the original atomic densities at the positions of the molecule to the actual density of that molecule. This atomic or so-called *promolecular* density is defined as the sum of the (spherically averaged) ground-state atomic densities $\sum_i \rho_i(\mathbf{r})$. This is the fictitious state in which the charge density has not been affected by chemical bonding and in which all atoms have zero charge. Q in Equation S4 then represents the amount of charge that, due to chemical bonding, flows to a position closer to nucleus A ($Q < 0$) or to a position further away from nucleus A ($Q > 0$).

[S9] (a) C. Nieuwland, P. Vermeeren, F. M. Bickelhaupt and C. Fonseca Guerra, *J. Comput. Chem.,* 2023, **44**, 2108; (b) C. Fonseca Guerra, J. W. Handgraaf, E. J. Baerends and F. M. Bickelhaupt, *J. Comput. Chem.,* 2004, **25**, 189; (c) O. A. Stasyuk, H. Szatylowicz, T. M. Krygowski and C. Fonseca Guerra, *Phys. Chem. Chem. Phys.,* 2016, **18**, 11624.

Data S1. Formaldehyde–X-urea complexes (X = O, S, Se)

Table S1. Decomposition of the hydrogen-bond energy ΔE (in kcal mol^{-1}) of the formaldehyde–1-monosubstituted X-urea (X = O, S, or Se) complexes.[a,b,c]

R^1	R^3	X	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
H	H	O	–5.2	0.4	–5.6	–7.0	5.6	–2.7	–1.6
		S	–6.3	0.5	–6.8	–8.4	6.9	–3.6	–1.7
		Se	–6.8	0.3	–7.1	–9.0	7.6	–3.9	–1.8
Cyclohexyl	H	O	–5.1	0.3	–5.4	–6.7	6.1	–2.8	–2.0
		S	–6.0	0.3	–6.3	–7.9	7.4	–3.5	–2.2
		Se	–6.4	0.2	–6.6	–8.5	7.9	–3.9	–2.2
Ph	H	O	–7.1	0.3	–7.5	–8.4	8.4	–3.6	–3.9
		S	–7.6	0.4	–8.0	–8.9	9.1	–3.9	–4.3
		Se	–7.7	0.4	–8.2	–9.7	10.1	–4.6	–3.9
3-(CF_3)C_6H_4	H	O	–8.0	0.3	–8.3	–9.5	8.7	–4.7	–2.9
		S	–8.5	0.5	–9.0	–10.4	9.7	–5.2	–3.1
		Se	–8.7	0.5	–9.2	–10.8	10.1	–5.4	–3.1
3,5-(CF_3)$_2C_6H_3$	H	O	–8.4	0.4	–8.7	–10.0	8.8	–4.9	–2.7
		S	–8.7	0.7	–9.4	–10.8	9.8	–5.4	–3.0
		Se	–8.9	0.7	–9.6	–11.1	10.3	–5.7	–3.1

[a] All computed at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] $\Delta E = \Delta E_{strain} + \Delta E_{int}$; $\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp}$ (see Method S2 for details). [c] See Figure 2 in the main text for the corresponding structures.

Table S2. Decomposition of the hydrogen-bond energy ΔE (in kcal mol^{-1}) of the symmetric formaldehyde–1,3-disubstituted X-urea (X = O, S, or Se) complexes.[a,b,c]

R^1	R^3	X	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
H	H	O	–5.2	0.4	–5.6	–7.0	5.6	–2.7	–1.6
		S	–6.3	0.5	–6.8	–8.4	6.9	–3.6	–1.7
		Se	–6.8	0.3	–7.1	–9.0	7.6	–3.9	–1.8
Cyclohexyl	Cyclohexyl	O	–5.0	0.3	–5.3	–6.5	6.2	–2.8	–2.2
		S	–6.0	0.1	–6.1	–7.7	7.5	–3.5	–2.4
		Se	–6.3	0.1	–6.4	–8.2	8.1	–3.8	–2.5
Ph	Ph	O	–7.8	0.1	–7.9	–9.5	8.6	–4.4	–2.6
		S	–7.2	0.6	–7.8	–9.6	9.0	–4.6	–2.7
		Se	–7.2	0.5	–7.7	–9.7	9.2	–4.6	–2.6
3-(CF_3)C_6H_4	3-(CF_3)C_6H_4	O	–9.7	0.2	–9.9	–11.3	9.6	–5.4	–2.7
		S	–9.1	1.3	–10.4	–12.0	10.6	–5.9	–3.1
		Se	–8.9	0.8	–9.7	–11.6	10.3	–5.6	–2.8
3,5-(CF_3)$_2C_6H_3$	3,5-(CF_3)$_2C_6H_3$	O	–10.6	0.2	–10.8	–12.2	10.0	–5.9	–2.7
		S	–9.7	1.1	–10.8	–12.4	10.6	–6.1	–2.9
		Se	–9.5	0.7	–10.2	–12.1	10.4	–5.9	–2.7

[a] All computed at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] $\Delta E = \Delta E_{strain} + \Delta E_{int}$; $\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp}$ (see Method S2 for details). [c] See Figure 3 in the main text for the corresponding structures.

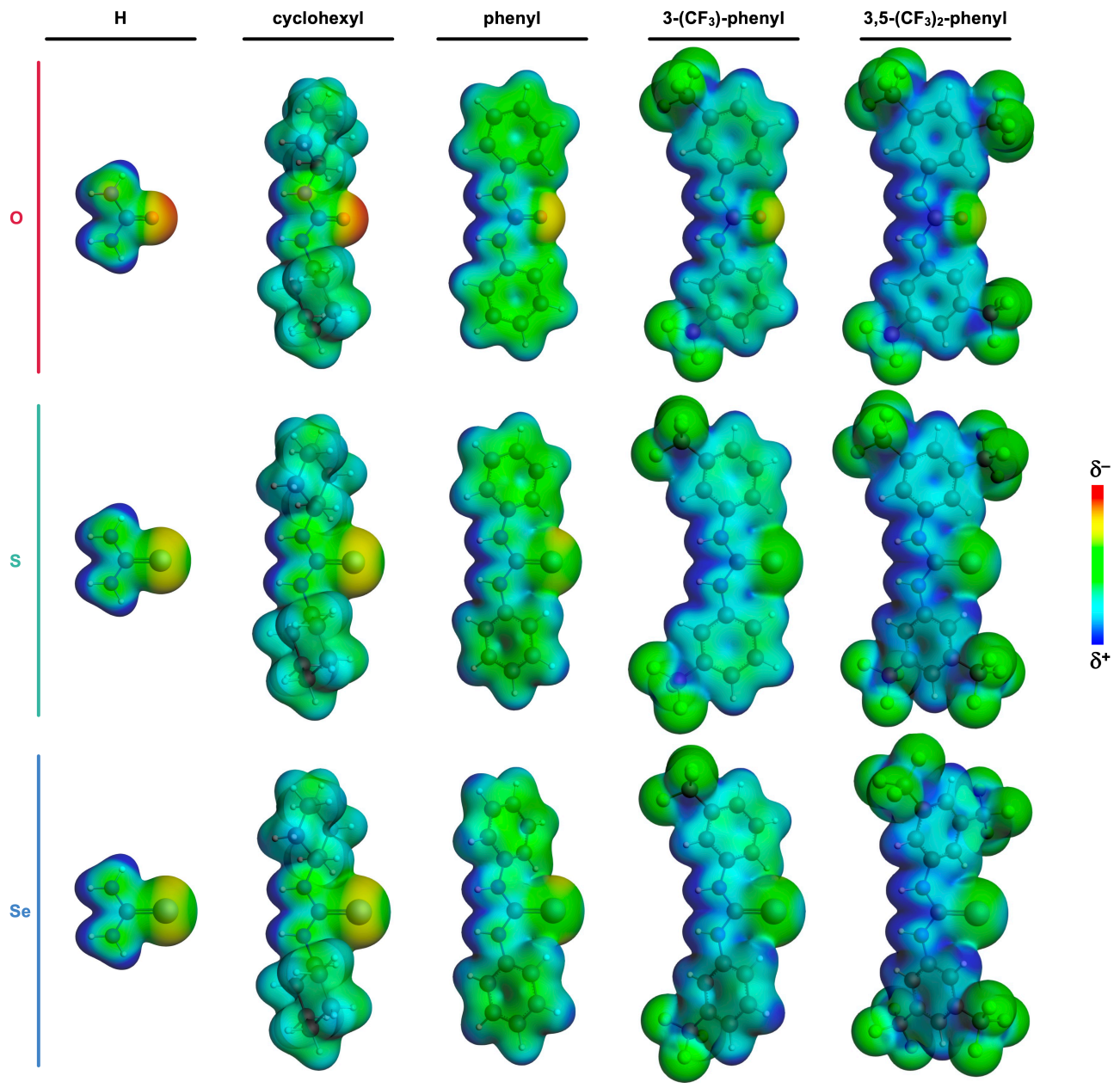
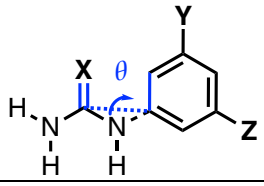


Figure S1. Molecular electrostatic potential surfaces (at 0.01 a.u.) from −0.1 (red) to +0.1 (blue) a.u. of the isolated 1,3-disubstituted X-urea derivatives (X = O, S, or Se; $R^1 = R^3$) in the geometry of the hydrogen-bonded complex with formaldehyde.

Data S2. Geometries of the (di)aryl substituted X-urea derivatives (X = O, S, Se)

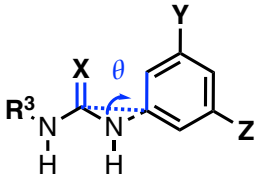
Table S3. XC–$C_{Ar}C_{Ar}$ dihedral angle θ (in degrees; highlighted in blue below) of the 1-aryl monosubstituted X-urea derivatives (X = O, S, or Se) in the equilibrium geometry of the X-urea monomer ($\theta_{monomer}$) and that of the hydrogen-bonded complex with formaldehyde ($\theta_{complex}$).[a]



X	Y	Z	$\theta_{monomer}$	$\theta_{complex}$	$\Delta\theta_{monomer\rightarrow complex}$[b]
O	H	H	6.0	3.0	–3.0
S			25.6	1.8	–23.8
Se			30.8	12.1	–18.7
O	H	CF_3	5.4	0.7	–4.7
S			23.0	4.4	–18.6
Se			32.4	7.5	–24.9
O	CF_3	CF_3	6.8	0.1	–6.7
S			34.0	3.1	–30.9
Se			35.9	15.3	–20.6

[a] Optimized at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] Change in θ going from the equilibrium geometry of the monomer to that of the hydrogen-bonded complex with formaldehyde (see Figure 2 in the main text for the corresponding structures).

Table S4. XC–$C_{Ar}C_{Ar}$ dihedral angle θ (in degrees; highlighted in blue below) of the 1,3-diaryl symmetrically disubstituted X-urea derivatives (X = O, S, or Se) in the equilibrium geometry of the X-urea monomer ($\theta_{monomer}$) and that of the hydrogen-bonded complex with formaldehyde ($\theta_{complex}$).[a]



X	R^3	Y	Z	$\theta_{monomer}$	$\theta_{complex}$	$\Delta\theta_{monomer\rightarrow complex}$[b]
O	Ph	H	H	0.6	0.1	–0.5
S				38.0	24.4	–13.6
Se				42.6	34.5	–8.1
O	3-$(CF_3)C_6H_4$	H	CF_3	1.6	0.4	–1.2
S				38.5	6.3	–32.2
Se				41.6	28.6	–13.0
O	3,5-$(CF_3)_2C_6H_3$	CF_3	CF_3	2.6	1.0	–1.6
S				40.0	21.7	–18.3
Se				43.4	35.9	–7.5

[a] Optimized at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] Change in θ going from the equilibrium geometry of the monomer to that of the hydrogen-bonded complex with formaldehyde (see Figure 3 in the main text for the corresponding structures).

Data S3. Asymmetric formaldehyde–1,3-disubstituted X-urea complexes (X = O, S, Se)

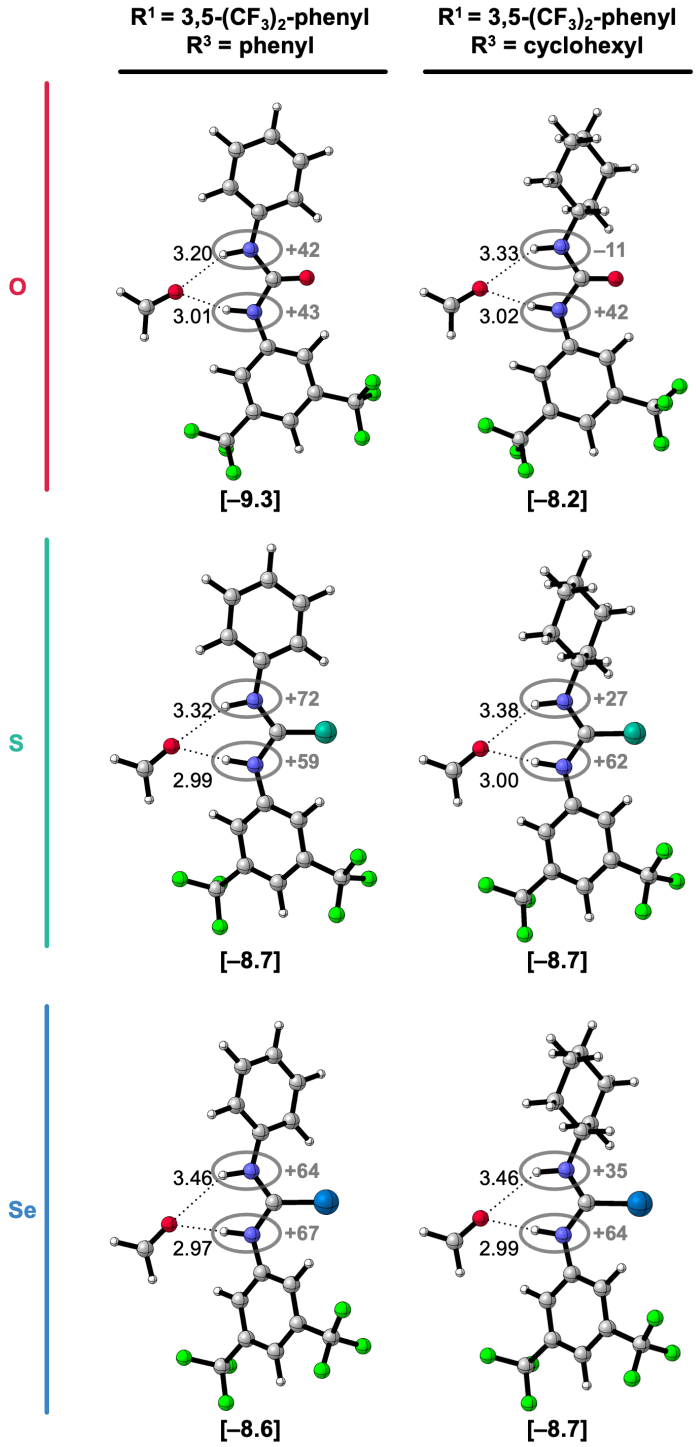


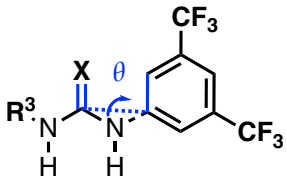
Figure S2. Equilibrium hydrogen-bonded complexes of formaldehyde with asymmetrically 1,3-disubstituted X-urea derivatives (X = O, S, or Se; $R^1 \neq R^3$). The equilibrium hydrogen-bond (O···(H)N) distances (in Å) are indicated and the hydrogen-bond energies ΔE (in kcal mol^{-1}) are shown below the structures between square brackets. The total Voronoi deformation density (VDD) atomic charge Q_{NH} of the NH groups (in milli-electrons) of the isolated X-urea in the geometry of the hydrogen-bonded complex is highlighted in grey. Color code of the ball-and-stick structures: H = white; C = grey; N = dark blue; O = pink; F = green; S = turquoise; Se = light blue.

Table S5. Decomposition of the hydrogen-bond energy ΔE (in kcal mol^{-1}) of the asymmetric formaldehyde–1,3-disubstituted X-urea (X = O, S, or Se) complexes.[a,b,c]

R^1	R^3	X	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
3,5-$(CF_3)_2C_6H_3$	Ph	O	–9.3	0.2	–9.5	–10.8	9.6	–5.3	–2.9
		S	–8.7	1.1	–9.8	–11.1	10.6	–5.8	–3.5
		Se	–8.6	0.8	–9.3	–10.8	10.5	–5.6	–3.5
3,5-$(CF_3)_2C_6H_3$	Cyclohexyl	O	–8.2	0.2	–8.4	–9.6	8.9	–4.8	–3.0
		S	–8.7	0.4	–9.1	–10.4	10.0	–5.3	–3.4
		Se	–8.7	0.5	–9.2	–10.6	10.3	–5.5	–3.4

[a] All computed at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] $\Delta E = \Delta E_{strain} + \Delta E_{int}$; $\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp}$ (see Method S2 for details). [c] See Figure S2 for the corresponding structures.

Table S6. XC–$C_{Ar}C_{Ar}$ dihedral angle θ (in degrees; highlighted in blue below) of the aromatic 1,3-asymmetrically disubstituted X-urea derivatives (X = O, S, or Se) in the equilibrium geometry of the X-urea monomer ($\theta_{monomer}$) and that of the hydrogen-bonded complex with formaldehyde ($\theta_{complex}$).[a]



X	R^3	$\theta_{monomer}$	$\theta_{complex}$	$\Delta\theta_{monomer\rightarrow complex}$[b]
O	Ph[c]	1.4 (0.6)	0.8 (0.1)	–0.6 (–0.5)
S		41.1 (35.9)	30.0 (4.8)	–11.1 (–31.1)
Se		43.5 (42.5)	34.3 (34.7)	–9.2 (–7.8)
O	cyclohexyl	5.9	1.1	–4.8
S		37.5	24.0	–13.5
Se		41.0	31.0	–10.0

[a] Optimized at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] Change in θ going from the equilibrium geometry of the monomer to that of the hydrogen-bonded complex with formaldehyde (see Figure S2 for the corresponding structures). [c] The dihedral angle θ' (in degrees) of the phenyl substituent (*i.e.,* R^3 = Ph) is denoted in between parentheses.

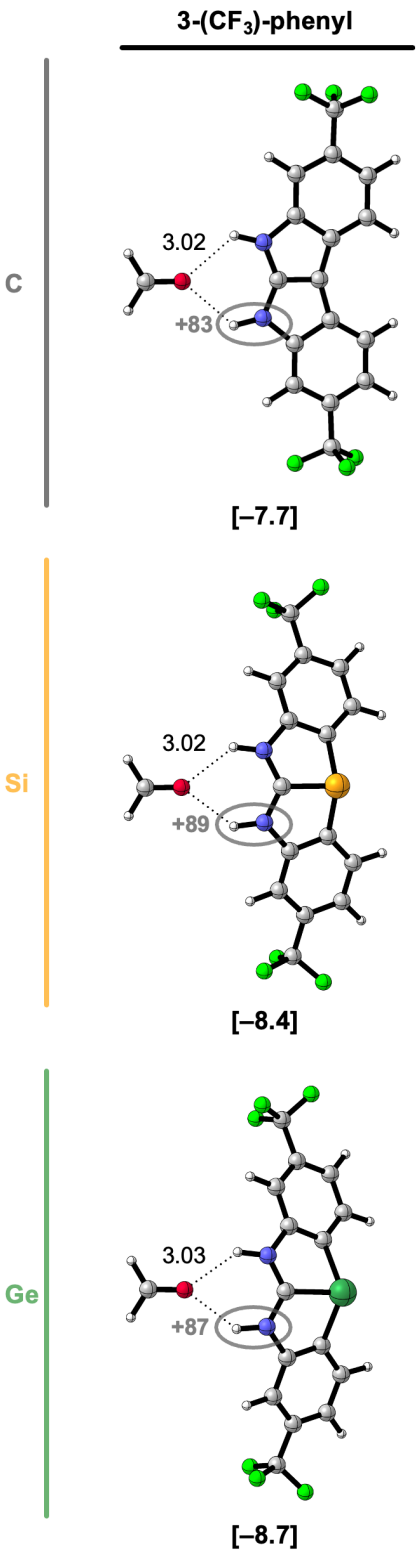
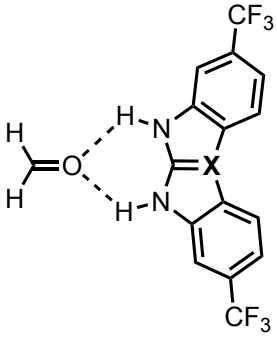


Figure S3. Equilibrium hydrogen-bonded complexes of formaldehyde with 1,3-(3-CF_3-phenyl)-disubstituted predistorted X-urea derivatives (X = C, Si, or Ge). The equilibrium hydrogen-bond (O···(H)N) distances (in Å) are indicated and the hydrogen-bond energies ΔE (in kcal mol^{-1}) are shown below the structures between square brackets. The total Voronoi deformation density (VDD) atomic charge Q_{NH} of the NH groups (in milli-electrons) of the isolated X-urea in the geometry of the hydrogen-bonded complex is highlighted in grey. Color code of the ball-and-stick structures: H = white; C = grey; N = dark blue; O = pink; F = green; Si = yellow; Ge = dark green.

Table S7. Decomposition of the hydrogen-bond energy ΔE (in kcal mol^{-1}) of the formaldehyde–1,3-disubstituted predistorted X-urea (X = C, Si, or Ge) complexes.[a,b,c]



X	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
C	–7.7	0.3	–8.0	–8.7	5.8	–3.0	–2.1
Si	–8.4	0.3	–8.7	–10.1	7.7	–4.1	–2.3
Ge	–8.7	0.2	–8.9	–10.6	8.4	–4.4	–2.3

[a] All computed at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] $\Delta E = \Delta E_{strain} + \Delta E_{int}$; $\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp}$. [c] See Figure S3 for the corresponding structures.

Data S5. 1,3-bis[3-(CF_3)phenyl]urea vs. 1,3-bis[4-(CF_3)phenyl]urea

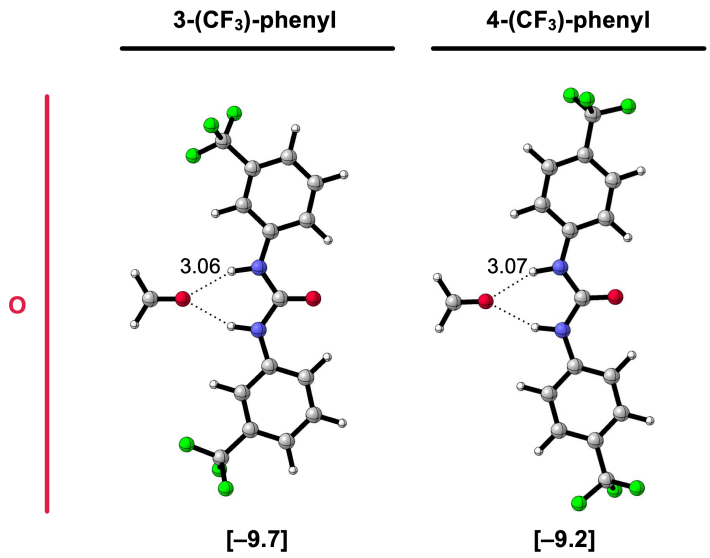


Figure S4. Equilibrium hydrogen-bonded complexes of formaldehyde with 1,3-[*n*-(CF_3)$_2$phenyl]urea [X = O; *n* = 3 (*meta*) or 4 (*para*)]. The equilibrium hydrogen-bond (O···(H)N) distances (in Å) are indicated and the hydrogen-bond energies ΔE (in kcal mol^{-1}) are shown below the structures between square brackets. Color code of the ball-and-stick structures: H = white; C = grey; N = blue; O = pink; F = green.

Table S8. Decomposition of the hydrogen-bond energy ΔE (in kcal mol^{-1}) of the formaldehyde–1,3-[*n*-(CF_3)$_2$phenyl]urea [X = O; *n* = 3 (*meta*) or 4 (*para*)] complexes.[a,b,c]

R^1	R^3	X	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
3-(CF_3)C_6H_4	3-(CF_3)C_6H_4	O	–9.7	0.2	–9.9	–11.3	9.6	–5.4	–2.7
4-(CF_3)C_6H_4	4-(CF_3)C_6H_4	O	–9.2	0.1	–9.3	–10.8	9.2	–5.1	–2.6

[a] All computed at ZORA-BLYP-D3(BJ)/TZ2P in C_1 symmetry. [b] $\Delta E = \Delta E_{strain} + \Delta E_{int}$; $\Delta E_{int} = \Delta V_{elstat} + \Delta E_{Pauli} + \Delta E_{oi} + \Delta E_{disp}$ (see Method S2 for details). [c] See Figure S4 for the corresponding structures.

Data S6. Cartesian coordinates and energies of optimized monomers

Below is a list consisting of the Cartesian coordinates (in Å), ADF total bond energies *E*, enthalpies *H*, Gibbs free energies *G* (in kcal mol^{-1}), and the number of imaginary frequencies (N_{imag}) of all optimized monomers reported in this work, optimized at the ZORA-BLYP-D3(BJ)/TZ2P level.

Formaldehyde

E: −494.36
H: −475.92
G: −491.92
N_{imag} = 0

H	1.17359952	0.94518045	−0.00137433
H	1.17359952	−0.94518045	−0.00137433
C	0.58285140	0.00000000	−0.00078141
O	−0.62895043	0.00000000	0.00043007

Urea

E: −1059.79
H: −1017.84
G: −1037.83
N_{imag} = 0

N	1.19058131	−0.51423267	−0.20589918
N	−1.10856075	−0.57298645	0.23787953
C	0.01965806	0.21608292	0.00597078
O	−0.01479062	1.44263088	−0.01017708
H	2.03030398	0.05252568	−0.15736625
H	−1.97879583	−0.05584540	0.17508885
H	1.27162565	−1.42924204	0.22558231
H	−1.13771448	−1.50223177	−0.16910903

Thiourea

E: −981.33
H: −940.56
G: −961.48
N_{imag} = 0

N	1.18058694	−0.48209422	−0.17255048
N	−1.10037175	−0.54121322	0.20366322
C	0.01918647	0.23320458	0.00580741
S	−0.02789530	1.90661262	−0.01635258
H	2.03215443	0.06588172	−0.16253884
H	−1.98139857	−0.04246125	0.17984260
H	1.25089122	−1.42476688	0.19942532
H	−1.11725683	−1.49590631	−0.14306214

Selenourea

E: −960.00
H: −919.61
G: −941.61
N_{imag} = 0

N	1.18308681	−0.47556264	−0.14830592
N	−1.10327084	−0.53548190	0.17917930
C	0.01949367	0.22112692	0.00591295
Se	−0.03210354	2.06244690	−0.01833854
H	2.03530979	0.07029821	−0.15012574
H	−1.98490549	−0.03868044	0.16719893
H	1.25510632	−1.44235687	0.15519136
H	−1.12048046	−1.51259614	−0.09820320

1-Cyclohexylurea

E: −3083.77
H: −2946.20
G: −2975.80
N_{imag} = 0

N	8.23146854	6.13271249	−14.31365898
N	10.03288949	4.86140649	−13.52989913
C	9.34282615	5.37353498	−14.64077448
H	4.56513732	5.07251824	−17.00449070
O	9.70001496	5.14557105	−15.79660773
H	5.81742183	6.08331274	−17.72290031
H	3.90175003	6.91551309	−15.46954316
H	10.95279432	4.51066520	−13.77681244
H	7.84907784	6.00952246	−13.38069314
H	10.02035813	5.41073956	−12.67550539
H	3.85204588	7.49109724	−17.13670227
C	7.27308715	6.54444426	−15.35011753
C	5.51482183	8.27549243	−15.96938790
C	6.52831832	7.81446984	−14.90307402
C	6.28437396	5.41639786	−15.71573367
C	5.27715937	5.87875579	−16.78638088
C	4.52960063	7.15084143	−16.34285317
H	7.87680383	6.77320882	−16.23606782
H	6.06240918	8.58940980	−16.87073187
H	4.97035361	9.15765041	−15.60881060
H	5.99297942	7.60375385	−13.96258059
H	7.25489196	8.60807972	−14.68852301
H	5.74119649	5.11626054	−14.80537702
H	6.85009169	4.54462163	−16.06307237

1-Cyclohexylthiourea

E: −3006.43
H: −2870.05
G: −2900.37
N_{imag} = 0

N	8.22872046	6.05720767	−14.37802963
N	10.05384571	4.93469487	−13.52208257
C	9.37498153	5.37077167	−14.64916197
H	4.51225551	5.09968755	−17.01779367
S	9.94551285	5.02990762	−16.19447427
H	5.76992839	6.10093544	−17.74031108
H	3.90142656	6.92933686	−15.44540894
H	10.98516398	4.58276233	−13.71271600
H	7.88370471	6.02944666	−13.42200312
H	9.96302611	5.47073021	−12.66222879
H	3.83549278	7.53125568	−17.10257450
C	7.26437532	6.50577876	−15.39163534

C	5.52741898	8.27214202	−15.95039586
C	6.55112998	7.78009615	−14.90769513
C	6.25500859	5.39610410	−15.75167216
C	5.23995308	5.89145968	−16.79925903
C	4.51948827	7.16805440	−16.32473702
H	7.85897659	6.73510667	−16.28359111
H	6.06576310	8.59167795	−16.85501193
H	5.00293039	9.15651601	−15.56683664
H	6.02822815	7.56456055	−13.96113451
H	7.29426268	8.55946298	−14.69684818
H	5.72282276	5.09095489	−14.83691370
H	6.80543455	4.52412212	−16.12134939

1-Cyclohexylselenourea

E: −2985.75
H: −2849.72
G: −2881.02
N_{imag} = 0

N	8.22088023	6.04199606	−14.37863517
N	10.06859418	4.95316075	−13.53356372
C	9.37669739	5.38637301	−14.63968082
H	4.50029699	5.10178613	−17.01327532
Se	10.02611144	5.03547053	−16.33844884
H	5.76432739	6.09396365	−17.73741190
H	3.89894518	6.93871757	−15.44546561
H	11.00132522	4.60445613	−13.72064374
H	7.88583672	6.04572627	−13.41770490
H	9.93586017	5.42123554	−12.63992591
H	3.83729370	7.53702655	−17.10405246
C	7.25731168	6.49728107	−15.39150538
C	5.53255719	8.27136396	−15.95313042
C	6.55330223	7.77645686	−14.90867114
C	6.24380619	5.39123713	−15.74738417
C	5.23221559	5.89004057	−16.79646933
C	4.51880647	7.17178388	−16.32505225
H	7.85450280	6.72009358	−16.28381122
H	6.07342230	8.58540203	−16.85804165
H	5.01301813	9.15956472	−15.57188416
H	6.02926164	7.56673558	−13.96133741
H	7.30132479	8.55206785	−14.70109740
H	5.70998765	5.08950336	−14.83248118
H	6.79188500	4.51725699	−16.11624676

1-Phenylurea

E: −2572.45
H: −2478.37
G: −2506.29
N_{imag} = 0

N	1.18494757	−0.86116706	−0.18403123
N	−1.09429938	−0.39563189	−0.15025547
C	0.19384051	0.12756729	−0.08840853
C	−2.32956230	0.28864858	−0.08678747
C	−2.43955252	1.67043429	0.15002307
C	−3.70749621	2.25616177	0.21089530
C	−4.86927995	1.49705472	0.03953504
C	−4.75510841	0.12237193	−0.19754018
C	−3.49806222	−0.47797955	−0.26029246
O	0.46628337	1.32147447	−0.00756059
H	−3.41718291	−1.54912950	−0.44402401
H	−5.64565903	−0.48696269	−0.33472631
H	−3.78113546	3.32613629	0.39382171
H	2.10853419	−0.50252154	0.03490497

H	0.99535594	−1.77876570	0.20732625
H	−1.17005236	−1.38441364	−0.36146645
H	−1.54245050	2.26230425	0.27442225
H	−5.84826550	1.96719920	0.08843030

1-Phenylthiourea

E: −2492.34
H: −2400.07
G: −2427.07
N_{imag} = 0

N	1.14711257	−0.89746257	−0.10323254
N	−1.07260590	−0.33905566	−0.05767201
C	0.21430901	0.12569699	−0.21617699
C	−2.31973878	0.33327965	−0.04365836
C	−2.47303444	1.68702371	0.29501868
C	−3.75313153	2.24699525	0.32152200
C	−4.88556943	1.48210348	0.02408534
C	−4.73025614	0.13033388	−0.30287565
C	−3.45803623	−0.44005996	−0.33825500
S	0.69133046	1.68626119	−0.58334999
H	−3.34111942	−1.49097450	−0.60145335
H	−5.59815010	−0.48193562	−0.53665291
H	−3.86067127	3.29755954	0.58229009
H	2.10851262	−0.57584932	−0.10774049
H	0.95431143	−1.66414431	0.53709373
H	−1.16627425	−1.34980779	−0.10950201
H	−1.60154246	2.28820975	0.51786875
H	−5.87528187	1.93136208	0.04699812

1-Phenylselenourea

E: −2470.96
H: −2379.07
G: −2406.96
N_{imag} = 0

N	−5.28782393	−1.21310921	0.45076443
N	−3.28803396	−0.29198378	−0.16730199
C	−4.17578006	−0.50620865	0.85348627
C	−2.06445354	0.42613630	−0.21075575
C	−1.79931619	1.54466257	0.59301808
C	−0.58257256	2.21663647	0.45250328
C	0.37003403	1.79879904	−0.48293461
C	0.09542071	0.69150803	−1.29294584
C	−1.11321525	0.00733200	−1.15720448
Se	−3.98126321	−0.04175505	2.62446292
H	−1.32003136	−0.86191021	−1.78059026
H	0.82322432	0.35318938	−2.02674035
H	−0.38325877	3.08083271	1.08220975
H	−6.00525793	−1.31605224	1.15903112
H	−5.61706379	−1.13013632	−0.50844375
H	−3.44482973	−0.86037266	−0.99646557
H	−2.53034639	1.86859157	1.32265510
H	1.31358092	2.32981925	−0.58150769

1-[3-(trifluoromethyl)phenyl]urea

Global minimum conformer
E: −2967.31
H: −2869.10
G: −2901.48
N_{imag} = 0

N	−0.98601782	0.21674962	0.23102304
N	−3.17670547	−0.41161402	0.69660829
C	−2.26612757	0.64364133	0.58822818
C	3.82915065	0.25280447	−0.72873758
O	−2.57236914	1.80611255	0.83192370
F	4.66843045	0.91782394	−1.58271190
F	3.60886003	−0.98928037	−1.26961455
H	−4.13596992	−0.09578145	0.79116970
H	−0.83571663	−0.78538409	0.19479727
H	−3.05949827	−1.23054669	0.10866172
F	4.53921100	0.04839524	0.43425881
H	1.36623339	−0.77916706	−0.30774427
C	0.17268321	0.99546288	0.03489726
C	0.18607554	2.40101633	0.09806311
C	1.38204254	3.08648966	−0.12753432
C	2.56930269	2.41005807	−0.41342980
C	2.54850445	1.01085963	−0.47538466
C	1.36495570	0.30671354	−0.25167151
H	−0.72929399	2.93110130	0.32501760
H	1.38214949	4.17273608	−0.07825394
H	3.49196042	2.95343782	−0.59028419

Local minimum conformer
E: −2966.90
H: −2868.71
G: −2901.04
N_{imag} = 0

N	−0.98601782	0.21674962	0.23102304
N	−3.17670547	−0.41161402	0.69660829
C	−2.26612757	0.64364133	0.58822818
C	3.82915065	0.25280447	−0.72873758
O	−2.57236914	1.80611255	0.83192370
F	4.66843045	0.91782394	−1.58271190
F	3.60886003	−0.98928037	−1.26961455
H	−4.13596992	−0.09578145	0.79116970
H	−0.83571663	−0.78538409	0.19479727
H	−3.05949827	−1.23054669	0.10866172
F	4.53921100	0.04839524	0.43425881
H	1.36623339	−0.77916706	−0.30774427
C	0.17268321	0.99546288	0.03489726
C	0.18607554	2.40101633	0.09806311
C	1.38204254	3.08648966	−0.12753432
C	2.56930269	2.41005807	−0.41342980
C	2.54850445	1.01085963	−0.47538466
C	1.36495570	0.30671354	−0.25167151
H	−0.72929399	2.93110130	0.32501760
H	1.38214949	4.17273608	−0.07825394
H	3.49196042	2.95343782	−0.59028419

1-[3-(trifluoromethyl)phenyl]thiourea

Global minimum conformer
E: −2886.85
H: −2790.46
G: −2821.73
N_{imag} = 0

N	−0.96071793	0.18997918	0.15412652
N	−3.12466787	−0.38283818	0.62882461
C	−2.16223795	0.61172432	0.68866322
F	4.55940233	−0.35473008	0.56060975
S	−2.48729674	2.08273711	1.41283961
F	4.74878836	0.24424925	−1.54766542
F	3.54930124	−1.52432478	−1.00736022
H	−4.04872127	−0.08573811	0.92048649
H	−0.89271996	−0.81327004	0.00608075
H	−3.10336679	−1.04988925	−0.13845130
H	1.74044932	3.90430420	−0.41581909
H	−0.47465718	2.88801711	0.02283802

C	0.26544818	0.86353314	−0.04488884
C	1.40104245	0.05463559	−0.22665017
C	2.64544725	0.63320631	−0.47669312
C	2.78284076	2.02601344	−0.53899180
C	1.65046902	2.82223005	−0.36077658
C	0.39470548	2.26012194	−0.11914120
H	1.31145612	−1.02779478	−0.17596421
C	3.86454691	−0.24561013	−0.62286695
H	3.75314866	2.47303518	−0.73112589

Local minimum conformer
E: −2886.54
H: −2789.60
G: −2822.86
N_{imag} = 0

N	1.15093403	−0.90731841	−0.03967222
N	−1.07806389	−0.38234696	0.00062154
C	0.20370661	0.08479354	−0.22901987
C	−2.31679158	0.29819517	−0.04009061
C	−2.45337483	1.65172967	0.30397091
C	−3.72188585	2.23607133	0.28390889
C	−4.86039717	1.49872223	−0.06735822
C	−4.71730755	0.14919322	−0.39331912
C	−3.45657001	−0.44835708	−0.38351101
F	−2.82178528	4.19609806	1.33611177
C	−3.87000040	3.70536909	0.60894090
H	2.10987499	−0.58516558	−0.10249559
H	0.97833544	−1.62817785	0.65658504
H	−3.35144256	−1.49902423	−0.64997193
H	−1.17023012	−1.39443939	−0.00033726
H	−1.58374416	2.23306081	0.57659235
H	−5.83787240	1.97060888	−0.07735924
S	0.63115527	1.61208225	−0.75002971
F	−3.95393538	4.47007387	−0.53200335
F	−5.01214293	3.95936211	1.32849216
H	−5.58966187	−0.44048841	−0.66302472

1-[3-(trifluoromethyl)phenyl]selenourea

Global minimum conformer
E: −2865.41
H: −2768.83
G: −2802.83
N_{imag} = 0

N	−0.97390169	0.17540627	0.00946081
N	−3.19844933	−0.29675909	0.24918146
C	−2.20686559	0.64194098	0.39646532
F	4.33885539	−0.16708317	1.59000799
Se	−2.59278538	2.28269782	1.13313402
F	4.97978398	0.12586291	−0.49402451
F	3.68717017	−1.58031401	0.03297850
H	−4.13648747	0.02607227	0.45435371
H	−0.90687478	−0.83511092	−0.08753078
H	−3.11318916	−1.02835925	−0.45213386
H	1.80476114	3.80740800	−0.65177209
H	−0.45694013	2.80597897	−0.49302136
C	0.28131041	0.82865324	−0.05197539
C	1.42319460	0.03466129	0.13341738
C	2.69532842	0.60230958	0.03331404
C	2.84399370	1.96803207	−0.23799060
C	1.70158141	2.74890778	−0.42656974
C	0.42315903	2.19388125	−0.34374193
H	1.31983363	−1.02420830	0.35681986

C	3.91593706	−0.25051427	0.28266662
H	3.83429035	2.40658344	−0.31071060

Local minimum conformer
E: −2865.14
H: −2768.60
G: −2802.71
N_{imag} = 0

N	1.15397308	−0.87471012	−0.00058249
N	−1.08330188	−0.39369899	0.05648966
C	0.17864281	0.06018003	−0.24837569
C	−2.32476603	0.28618686	−0.01488818
C	−2.45710015	1.63424093	0.34768521
C	−3.71676946	2.23344604	0.29382836
C	−4.84924542	1.51133395	−0.10872067
C	−4.71032554	0.16559336	−0.44880844
C	−3.45524917	−0.44597644	−0.40627957
F	−2.81462875	4.17839597	1.37080776
C	−3.86585889	3.69679050	0.64230426
H	2.10526195	−0.55536075	−0.14043295
H	1.01489969	−1.57594775	0.72302409
H	−3.34866117	−1.49206723	−0.68854279
H	−1.17322521	−1.40295510	0.14633151
H	−1.59051560	2.19928116	0.66276260
H	−5.82105744	1.99384438	−0.14566347
Se	0.60746131	1.68354122	−0.99452668
F	−3.96004381	4.47894976	−0.48536107
F	−5.00470363	3.93567366	1.37330285
H	−5.57921057	−0.40987768	−0.75735461

1-[3,5-bis(trifluoromethyl)phenyl]urea

E: −3360.34
H: −3258.05
G: −3294.75
N_{imag} = 0

N	1.18104315	−0.84083017	−0.17069363
N	−1.10635984	−0.41665849	−0.14585107
C	0.18229727	0.12647749	−0.07121059
C	−2.33620403	0.26149402	−0.08137036
C	−2.44800600	1.63543085	0.19125432
C	−3.71720012	2.21895181	0.25235560
C	−4.88059489	1.47545301	0.04509787
C	−4.75676284	0.10890011	−0.22754961
C	−3.50328621	−0.49658041	−0.28961787
C	−6.00168361	−0.73239304	−0.39797946
C	−3.81180818	3.71066503	0.49906452
H	2.10688862	−0.48233659	0.03655775
H	1.00397223	−1.78224798	0.16362183
H	−3.43017542	−1.55980967	−0.50407039
H	−1.17318713	−1.40215554	−0.37492524
H	−1.55359284	2.22391986	0.34487237
H	−5.85614208	1.94468573	0.09294555
O	0.42415404	1.32393897	0.02432491
F	−7.01773437	−0.03924918	−0.99466793
F	−6.48215675	−1.17165465	0.81437873
F	−5.77476619	−1.85197665	−1.15602837
F	−2.89934093	4.13959556	1.42372952
F	−5.04898052	4.08656703	0.94758709
F	−3.57386303	4.42436977	−0.65156998

1-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −3279.74
H: −3178.73
G: −3216.28
N_{imag} = 0

N	1.14177741	−0.88213372	−0.05072534
N	−1.09319474	−0.39397766	0.06615654
C	0.17032402	0.07339743	−0.26863864
C	−2.33155767	0.28133747	0.02766360
C	−2.45789874	1.64697259	0.32885009
C	−3.72250791	2.23683311	0.31089826
C	−4.87107341	1.49657445	0.00912685
C	−4.73544919	0.13600672	−0.27213813
C	−3.47690168	−0.47116617	−0.26793991
C	−5.95911732	−0.71111290	−0.53854124
C	−3.85218356	3.72059388	0.58427249
H	2.09269227	−0.56460110	−0.19761303
H	1.01267457	−1.57139754	0.68512391
H	−3.38645888	−1.52765476	−0.50795428
H	−1.17664241	−1.40533317	0.12252196
H	−1.58158402	2.23242170	0.57015044
H	−5.84686595	1.96826591	−0.00085044
S	0.52938978	1.56146725	−0.93099415
F	−7.01548359	0.02426603	−0.99334616
F	−6.38311373	−1.35325363	0.60329323
F	−5.71548410	−1.69158862	−1.46612038
F	−2.84276389	4.19526112	1.37442278
F	−5.03316026	4.02560977	1.20894886
F	−3.82341006	4.44897153	−0.57999776

1-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −3258.31
H: −3157.69
G: −3196.02
N_{imag} = 0

N	1.14254632	−0.86615821	−0.02684356
N	−1.09348564	−0.39440086	0.09232798
C	0.16011654	0.06003906	−0.25867270
C	−2.33495797	0.27970219	0.04684137
C	−2.45989720	1.64387347	0.35232387
C	−3.72221990	2.23731881	0.31923037
C	−4.86830420	1.49946583	0.00015550
C	−4.73370869	0.13922143	−0.28079890
C	−3.47571573	−0.47119842	−0.26292424
C	−5.95510973	−0.70572629	−0.56258007
C	−3.85561503	3.71987500	0.59591558
H	2.09033092	−0.55893733	−0.20922696
H	1.02200155	−1.58338154	0.68370842
H	−3.38356201	−1.52698039	−0.50523154
H	−1.17802303	−1.40274355	0.19700903
H	−1.58434492	2.22440101	0.60869670
H	−5.84284935	1.97363148	−0.02136446
Se	0.55709829	1.67367894	−1.04052413
F	−7.01246146	0.03395247	−1.00728671
F	−6.37903052	−1.36719448	0.56844510
F	−5.70737857	−1.67113832	−1.50490045
F	−2.82988647	4.20292733	1.35854156
F	−5.02271529	4.01488481	1.25193380
F	−3.86526838	4.44779574	−0.56880436

1,3-Dicyclohexylurea

E: −5107.43
H: −4874.29
G: −4913.45
N_{imag} = 0

N	2.94169612	−0.64143172	0.53965770
N	0.71154619	−0.19633054	0.00255798
C	1.88750428	0.26799830	0.58777661
H	5.11020146	−2.24427355	0.69878214
H	5.09322336	−0.88523446	4.68071369
H	5.47902902	−0.84280471	−0.31437620
H	3.67241308	−1.86181948	2.87796595
O	1.98648287	1.38521433	1.10279357
H	5.46994137	0.50494268	3.66487019
H	6.26340362	−2.40869504	3.09884148
H	3.12731454	−0.21535358	3.24007324
H	−3.83128286	0.32075955	−0.74342293
H	2.69044271	−1.61705291	0.40520752
H	0.80954738	−0.95751157	−0.66384666
H	7.35759139	−1.11348102	3.58734056
C	4.15170879	−0.41308169	1.34316398
C	6.63194825	−0.94700726	1.54038805
C	5.34228055	−1.16672603	0.72485992
C	3.95738932	−0.79864241	2.82588711
C	5.24612600	−0.57216249	3.63982215
C	6.44037586	−1.32464110	3.02222307
H	4.34179777	0.66519032	1.29102924
H	6.92128613	0.11254655	1.47294603
H	7.45430814	−1.52627234	1.10100021
C	−2.66791199	1.75256859	−1.90803028
H	−1.64792787	−0.78369613	−1.17315790
H	−1.15988928	3.08978367	−2.74249970
H	−1.88166114	−0.59928476	0.56981338
H	−0.02213416	0.89712753	−2.39627742
H	−1.40357279	3.26569153	−1.00581102
H	−2.64280905	1.09176663	−2.78841355
H	0.77676426	2.14322103	−1.42254630
H	−3.50402060	2.44790677	−2.05855681
C	−0.39448103	0.73332785	−0.27060405
C	−2.90596833	0.90290486	−0.64452661
C	−1.72084360	−0.04146986	−0.36110525
C	−0.15496388	1.57864772	−1.54060779
C	−1.33836787	2.52591665	−1.81781311
H	−0.43098382	1.41045531	0.59060872
H	−3.04463364	1.57138458	0.21850596

1,3-Dicyclohexylthiourea

E: −5030.67
H: −4798.75
G: −4838.59
N_{imag} = 0

N	2.92201346	−0.48767717	0.66657360
N	0.76994553	−0.00402649	0.01750933
C	1.90093920	0.43011076	0.66347672
H	5.01315831	−2.19282221	0.66723876
H	5.18131009	−1.02637942	4.70905342
H	5.41753074	−0.75874879	−0.28811218
H	3.66107000	−1.85158496	2.91045551
S	2.02477712	1.95169072	1.38691141
H	5.58969713	0.39209357	3.74582231
H	6.22977992	−2.52484002	3.02126422
H	3.20576964	−0.19893599	3.36397033

H	−3.78408171	0.16992100	−0.78415219
H	2.69041789	−1.43734000	0.38525707
H	0.85596447	−0.84306723	−0.55103864
H	7.39801093	−1.30505888	3.53177830
C	4.16642940	−0.35070928	1.43449822
C	6.61885277	−1.00899965	1.52039118
C	5.29596212	−1.12921432	0.73756652
C	3.99419661	−0.80156723	2.90008102
C	5.31667429	−0.67162081	3.67931759
C	6.45469233	−1.44746503	2.98870937
H	4.40353535	0.71919338	1.42835740
H	6.95574581	0.03792241	1.49192020
H	7.39801882	−1.60432180	1.02732160
C	−2.70836341	1.65275152	−1.96970521
H	−1.52608816	−0.79081510	−1.16151998
H	−1.28599373	3.07131358	−2.81992476
H	−1.79372886	−0.57767784	0.57506174
H	−0.00379873	0.97027816	−2.41006616
H	−1.56034887	3.26948136	−1.09013593
H	−2.62768171	0.97538361	−2.83402756
H	0.69510907	2.29068261	−1.45499703
H	−3.58870366	2.28476714	−2.14467944
C	−0.39502310	0.83753060	−0.28499569
C	−2.90328288	0.81782671	−0.68905636
C	−1.65941202	−0.03529988	−0.36929577
C	−0.19391584	1.66177343	−1.57382533
C	−1.43636513	2.51800765	−1.88409480
H	−0.48707059	1.53200424	0.55772289
H	−3.09839158	1.49411194	0.15646013

1,3-Dicyclohexylselenourea

E: −5010.40
H: −4778.80
G: −4819.57
N_{imag} = 0

N	2.91298434	−0.48487047	0.69239822
N	0.78267925	0.01669731	−0.00048797
C	1.90100497	0.42787181	0.66156772
H	5.01326834	−2.18141914	0.66066838
H	5.19100071	−1.05896682	4.71573532
H	5.40691458	−0.73295300	−0.27879897
H	3.66718721	−1.87277744	2.91474816
Se	2.03590427	2.10430280	1.46084376
H	5.58687958	0.37237165	3.76629408
H	6.24124113	−2.53308138	3.00759715
H	3.20626016	−0.22589789	3.38642077
H	−3.77833719	0.16659408	−0.76816298
H	2.70987559	−1.42241539	0.35189097
H	0.83997762	−0.85569795	−0.52184824
H	7.40456383	−1.31220639	3.52652261
C	4.16217131	−0.35217241	1.45486727
C	6.61608538	−0.99880741	1.52179239
C	5.29075082	−1.11713193	0.74255158
C	3.99554116	−0.82129887	2.91449593
C	5.32034887	−0.69220699	3.68951040
C	6.45982946	−1.45412579	2.98585931
H	4.39306566	0.71942254	1.46084575
H	6.94706226	0.05010520	1.50325315
H	7.39611701	−1.58468974	1.01900750
C	−2.71614320	1.64455446	−1.97214358
H	−1.52075968	−0.79067786	−1.15489297
H	−1.30450222	3.06121564	−2.84321383
H	−1.77608630	−0.56360019	0.58258387

H	−0.01225871	0.96691458	−2.42932316
H	−1.56504776	3.27034952	−1.11252097
H	−2.64049161	0.96149938	−2.83244356
H	0.68897326	2.29590388	−1.48642462
H	−3.59967514	2.27282160	−2.14430297
C	−0.38984173	0.85011394	−0.30038182
C	−2.89905863	0.81801061	−0.68427890
C	−1.65022575	−0.02922282	−0.36759414
C	−0.19879616	1.66351725	−1.59664678
C	−1.44601643	2.51402613	−1.90250038
H	−0.47678959	1.55141927	0.53764573
H	−3.08952186	1.49938015	0.15806215

1,3-Diphenylurea

E: −4085.03
H: −3938.84
G: −3974.97
N_{imag} = 0

N	0.86627103	1.13945697	−0.45165770
N	−1.21068196	0.14554469	−0.67193359
C	−0.39850712	0.96513550	0.11610078
C	−2.54156078	−0.26678900	−0.43554385
C	−3.13166213	−1.10328361	−1.40363959
C	−4.44082268	−1.55603354	−1.24680899
C	−5.18618316	−1.18337008	−0.12219772
C	−4.59885715	−0.35313107	0.83724605
C	−3.28734225	0.11013136	0.69591208
C	1.95769988	1.89083000	0.03960543
C	3.13592658	1.88404589	−0.73299065
C	4.25902586	2.59950169	−0.32041820
C	4.22870456	3.33521287	0.86997618
C	3.05846932	3.34094087	1.63506969
C	1.92306489	2.62927602	1.23624968
H	3.02006846	3.90832427	2.56258496
H	−2.55817451	−1.39826693	−2.28229807
O	−0.75271150	1.47038422	1.17690315
H	1.05279281	0.66705086	−1.32888302
H	−2.83806888	0.75233899	1.44108792
H	−0.81486165	−0.21347043	−1.53328129
H	−4.87745333	−2.20112322	−2.00597439
H	−6.20720354	−1.53518087	0.00226406
H	−5.16609972	−0.05518680	1.71653010
H	3.16815910	1.31352377	−1.66111021
H	5.15856405	2.58063886	−0.93164307
H	5.10323626	3.89379986	1.19387185
H	1.02076833	2.63678137	1.83239640

1,3-Diphenylthiourea

E: −4003.03
H: −3858.19
G: −3894.89
N_{imag} = 0

N	0.80577305	1.20105324	−0.39780870
N	−1.19000653	0.12703447	−0.55087866
C	−0.42356425	0.99526525	0.21879062
C	−2.55037124	−0.24395133	−0.41011562
C	−2.90707111	−1.55559809	−0.76707387
C	−4.24018880	−1.96619192	−0.70821331
C	−5.23155610	−1.07520267	−0.28413613
C	−4.87400891	0.23165994	0.06683778
C	−3.54544399	0.65667556	0.00171917
C	1.95295747	1.88171081	0.08091728

C	2.73152053	2.58234785	−0.85605090
C	3.90487337	3.22647722	−0.45911808
C	4.31021164	3.18601045	0.87900533
C	3.53537954	2.48351903	1.80910165
C	2.36569377	1.82647257	1.42157359
H	3.84516231	2.43868476	2.85081752
H	−2.13465968	−2.25565119	−1.08327927
S	−0.90432764	1.68316016	1.65932012
H	0.80798065	1.05743155	−1.40396821
H	−3.27722904	1.66956193	0.27364522
H	−0.65698368	−0.49724169	−1.15015288
H	−4.49977262	−2.98517621	−0.98586301
H	−6.26939135	−1.39441694	−0.22964021
H	−5.63762259	0.93541668	0.39054040
H	2.40958355	2.62819199	−1.89572647
H	4.49525241	3.76644768	−1.19578970
H	5.21905559	3.69357759	1.19262302
H	1.77236345	1.28432187	2.14672201

1,3-Diphenylselenourea

E: −3981.41
H: −3836.94
G: −3874.46
N_{imag} = 0

N	0.80052530	1.21148778	−0.41911726
N	−1.17827865	0.10971417	−0.54753586
C	−0.42048485	0.99730963	0.19271303
C	−2.54266847	−0.25610762	−0.40932793
C	−2.88836136	−1.59353439	−0.66065254
C	−4.22310253	−2.00015129	−0.59557343
C	−5.22268503	−1.07742684	−0.27109645
C	−4.87442368	0.25641888	−0.02709873
C	−3.54479072	0.67577107	−0.10002549
C	1.94950827	1.88933382	0.06628301
C	2.68500652	2.66504665	−0.84360776
C	3.85524077	3.30912194	−0.43458724
C	4.29583121	3.19082992	0.88737952
C	3.56258192	2.41120691	1.79000232
C	2.39786192	1.75449822	1.38876081
H	3.90195943	2.30579965	2.81796319
H	−2.10801722	−2.31592357	−0.89614717
Se	−0.95620064	1.78008237	1.76406683
H	0.81277964	1.05334630	−1.42391392
H	−3.27988594	1.70881318	0.08776095
H	−0.64453057	−0.52152360	−1.14037711
H	−4.47708044	−3.03970119	−0.78927438
H	−6.26138874	−1.39301498	−0.21134925
H	−5.64546331	0.98356560	0.21736571
H	2.33178007	2.77193900	−1.86828417
H	4.41422748	3.90998188	−1.14814625
H	5.20152817	3.69812560	1.21056604
H	1.83443354	1.15051270	2.08916626

1,3-bis[3-(trifluoromethyl)phenyl]urea

Global minimum conformer
E: −4874.27
H: −4720.35
G: −4762.50
N_{imag} = 0

N	0.00890112	1.15686929	0.21307243
N	−0.00890112	−1.15686929	0.21307243
C	0.00000000	−0.00000000	0.99695622

C	−0.02970946	−2.50164169	0.64047012
C	−0.00955867	−3.48574847	−0.36443999
C	−0.03730340	−4.83831815	−0.02569332
C	−0.08070345	−5.23695346	1.31654442
C	−0.09954517	−4.25474000	2.30779701
C	−0.07438641	−2.89437853	1.99046364
C	0.02970946	2.50164169	0.64047012
C	0.00955867	3.48574847	−0.36443999
C	0.03730340	4.83831815	−0.02569332
C	0.08070345	5.23695346	1.31654442
C	0.09954517	4.25474000	2.30779701
C	0.07438641	2.89437853	1.99046364
F	0.40223200	5.41401579	−2.32586054
H	0.02105562	−3.19480781	−1.41171317
O	0.00000000	0.00000000	2.22322074
H	−0.01888167	1.04122719	−0.79375932
H	−0.08975188	−2.14031407	2.76534906
H	0.01888167	−1.04122719	−0.79375932
C	0.03806153	−5.88266255	−1.11399635
H	−0.10483629	−6.29070427	1.57532529
F	0.70545294	6.99415194	−0.81951750
H	−0.02105562	3.19480781	−1.41171317
C	−0.03806153	5.88266255	−1.11399635
H	0.10483629	6.29070427	1.57532529
H	0.08975188	2.14031407	2.76534906
F	−0.70545294	−6.99415194	−0.81951750
F	−1.32967712	6.31816776	−1.31126526
H	0.13666425	4.54875664	3.35391455
H	−0.13666425	−4.54875664	3.35391455
F	1.32967712	−6.31816776	−1.31126526
F	−0.40223200	−5.41401579	−2.32586054

Local minimum conformer
E: −4873.44
H: −4719.50
G: −4761.99
N_{imag} = 0

N	0.01766460	1.15730684	1.29451410
C	0.00000000	0.00000000	0.51028436
H	0.05939637	1.04175103	2.30068133
C	0.02868485	2.50196845	0.86710663
N	−0.01766460	−1.15730684	1.29451410
O	0.00000000	0.00000000	−0.71649538
C	0.10102992	3.49258381	1.86581005
C	−0.03657502	2.88680169	−0.48219726
H	−0.05939637	−1.04175103	2.30068133
C	−0.02868485	−2.50196845	0.86710663
C	0.10816652	4.84293792	1.52500574
H	0.14993988	3.19902382	2.91377622
C	−0.03003286	4.24848396	−0.80268408
H	−0.09363264	2.13278586	−1.25448240
C	−0.10102992	−3.49258381	1.86581005
C	0.03657502	−2.88680169	−0.48219726
C	0.04414542	5.23584238	0.18549957
H	0.16250563	5.59384380	2.30910493
C	−0.04554718	4.65163109	−2.26088321
C	−0.10816652	−4.84293792	1.52500574
H	−0.14993988	−3.19902382	2.91377622
C	0.03003286	−4.24848396	−0.80268408
H	0.09363264	−2.13278586	−1.25448240
H	0.04582116	6.28644746	−0.08528292
F	−0.73498477	3.76793976	−3.04383241
F	−0.61151170	5.88586974	−2.45246258
F	1.22962895	4.72335623	−2.77656819

C	−0.04414542	−5.23584238	0.18549957
H	−0.16250563	−5.59384380	2.30910493
C	0.04554718	−4.65163109	−2.26088321
H	−0.04582116	−6.28644746	−0.08528292
F	0.73498477	−3.76793976	−3.04383241
F	0.61151170	−5.88586974	−2.45246258
F	−1.22962895	−4.72335623	−2.77656819

1,3-bis[3-(trifluoromethyl)phenyl]thiourea

Global minimum conformer
E: −4791.92
H: −4639.40
G: −4682.44
N_{imag} = 0

N	−1.05235146	0.38800767	0.21286455
N	1.11424986	−0.25328385	−0.03035825
C	0.24241359	0.55193196	0.69569145
C	2.48680287	−0.51270022	0.19690485
C	3.30656880	−0.68887851	−0.92728461
C	4.65751546	−1.00795081	−0.76734775
C	5.20979149	−1.13740177	0.51215591
C	4.38517252	−0.96360351	1.62673218
C	3.03060329	−0.66067550	1.48308411
C	−2.22400810	1.10811243	0.54702866
C	−3.43412271	0.40001844	0.57569130
C	−4.63231195	1.06975331	0.83709834
C	−4.63575129	2.44631016	1.09021490
C	−3.42587770	3.14454494	1.05701601
C	−2.22339108	2.49264394	0.78099668
F	−5.89221185	−0.84379428	0.13406212
H	2.89181026	−0.57703880	−1.92594841
S	0.67944694	1.55685306	1.94900895
H	−1.23245330	−0.50195957	−0.24413887
H	2.39945099	−0.53687315	2.35352676
H	0.80203634	−0.48797536	−0.96887492
C	5.53706586	−1.14590851	−1.98702525
H	6.26072707	−1.38035190	0.63234210
F	−7.00238292	1.02323761	0.50992169
H	−3.44176188	−0.67185063	0.39469435
C	−5.92096055	0.28620471	0.91215043
H	−5.56796565	2.96197597	1.29775893
H	−1.29324986	3.04516433	0.74835111
F	6.11891940	0.05271645	−2.33372754
F	4.83887929	−1.57063224	−3.08961522
F	6.56067335	−2.03396846	−1.79331250
F	−6.18855904	−0.13251946	2.19604567
H	−3.41838817	4.21639456	1.23800702
H	4.80005611	−1.07586923	2.62521000

Local minimum conformer
E: −4791.43
H: −4638.97
G: −4682.12
N_{imag} = 0

N	−0.34293673	1.08432017	−1.10752971
N	0.34293673	−1.08432017	−1.10752971
C	0.00000000	−0.00000000	−0.30381131
C	0.61951772	−2.41610833	−0.71644478
C	1.63423817	−3.10893038	−1.39425982
C	1.90765316	−4.44227406	−1.08222753
C	1.18131164	−5.09611507	−0.08653426

C	0.16289719	−4.40142677	0.58106607
C	−0.12777526	−3.07111448	0.27379454
C	−0.61951772	2.41610833	−0.71644478
C	−1.63423817	3.10893038	−1.39425982
C	−1.90765316	4.44227406	−1.08222753
C	−1.18131164	5.09611507	−0.08653426
C	−0.16289719	4.40142677	0.58106607
C	0.12777526	3.07111448	0.27379454
C	0.60653620	5.09999331	1.67914068
H	2.21543107	−2.59868767	−2.16058992
S	0.00000000	−0.00000000	1.35951249
H	−0.69572411	0.84214559	−2.02949583
H	−0.92167184	−2.54996263	0.79083550
H	0.69572411	−0.84214559	−2.02949583
F	−0.86629668	−6.41214006	1.36902848
H	1.39366982	−6.13055847	0.16474437
C	−0.60653620	−5.09999331	1.67914068
H	−2.21543107	2.59868767	−2.16058992
F	−0.09717151	5.11294048	2.86074280
H	−1.39366982	6.13055847	0.16474437
H	0.92167184	2.54996263	0.79083550
F	0.86629668	6.41214006	1.36902848
F	1.80953140	4.50543286	1.94293272
H	−2.69707577	4.96800586	−1.61305388
F	−1.80953140	−4.50543286	1.94293272
F	0.09717151	−5.11294048	2.86074280
H	2.69707577	−4.96800586	−1.61305388

1,3-bis[3-(trifluoromethyl)phenyl]selenourea

Global minimum conformer
E: −4770.22
H: −4618.08
G: −4661.54
N_{imag} = 0

N	0.04307034	1.13383157	0.10287065
N	−0.04307034	−1.13383157	0.10287065
C	−0.00000000	0.00000000	0.89381783
C	−0.26330441	−2.48222308	0.48024429
C	0.46520182	−3.47224754	−0.19209526
C	0.24373193	−4.82191437	0.09812817
C	−0.69031689	−5.19390507	1.07144733
C	−1.41535701	−4.19909346	1.73337168
C	−1.21718753	−2.84913895	1.44205479
C	0.26330441	2.48222308	0.48024429
C	−0.46520182	3.47224754	−0.19209526
C	−0.24373193	4.82191437	0.09812817
C	0.69031689	5.19390507	1.07144733
C	1.41535701	4.19909346	1.73337168
C	1.21718753	2.84913895	1.44205479
F	−1.46361978	5.48472753	−1.85439016
H	1.20466271	−3.19221728	−0.93798105
Se	−0.00000000	0.00000000	2.72675783
H	−0.34800639	1.02677762	−0.83025868
H	−1.79053713	−2.08475347	1.95108751
H	0.34800639	−1.02677762	−0.83025868
C	1.06947888	−5.87622705	−0.59931531
H	−0.85531469	−6.24253609	1.29768953
F	−0.39325481	7.05800880	−0.74123682
H	−1.20466271	3.19221728	−0.93798105
C	−1.06947888	5.87622705	−0.59931531
H	0.85531469	6.24253609	1.29768953
H	1.79053713	2.08475347	1.95108751
F	2.22132719	−6.16519100	0.09698607

F	1.46361978	−5.48472753	−1.85439016
F	0.39325481	−7.05800880	−0.74123682
F	−2.22132719	6.16519100	0.09698607
H	2.15444579	4.47847673	2.47986029
H	−2.15444579	−4.47847673	2.47986029

Local minimum conformer
E: −4769.87
H: −4618.39
G: −4659.94
N_{imag} = 0

N	−0.36617986	1.07527384	−1.09921521
N	0.36617986	−1.07527384	−1.09921521
C	0.00000000	0.00000000	−0.30846959
C	0.64474174	−2.40746676	−0.70248917
C	1.72129899	−3.07117116	−1.30664260
C	1.99906343	−4.40154165	−0.98122233
C	1.21366445	−5.07595940	−0.04670677
C	0.13150305	−4.40857215	0.54580910
C	−0.16230955	−3.08289968	0.22414635
C	−0.64474174	2.40746676	−0.70248917
C	−1.72129899	3.07117116	−1.30664260
C	−1.99906343	4.40154165	−0.98122233
C	−1.21366445	5.07595940	−0.04670677
C	−0.13150305	4.40857215	0.54580910
C	0.16230955	3.08289968	0.22414635
C	0.70474084	5.13409989	1.57486021
H	2.34801137	−2.54168079	−2.02206066
Se	0.00000000	0.00000000	1.52227600
H	−0.71325703	0.83633515	−2.02514650
H	−1.00445977	−2.57990586	0.67987972
H	0.71325703	−0.83633515	−2.02514650
F	−0.94306554	−6.43796941	1.21453744
H	1.42890822	−6.10734181	0.21506482
C	−0.70474084	−5.13409989	1.57486021
H	−2.34801137	2.54168079	−2.02206066
F	0.07685849	5.17909224	2.79742764
H	−1.42890822	6.10734181	0.21506482
H	1.00445977	2.57990586	0.67987972
F	0.94306554	6.43796941	1.21453744
F	1.92245539	4.54584119	1.77736505
H	−2.83777165	4.90721976	−1.45251029
F	−1.92245539	−4.54584119	1.77736505
F	−0.07685849	−5.17909224	2.79742764
H	2.83777165	−4.90721976	−1.45251029

1,3-bis[3,5-bis(trifluoromethyl)phenyl]urea
E: −5659.48
H: −5497.99
G: −5546.70
N_{imag} = 0

H	−2.82350257	−0.09103455	4.00078762
H	−4.91764024	−0.01792181	4.00079789
N	−5.02869591	−0.05799406	2.99385861
C	−3.87057700	−0.05443162	2.21039922
H	−7.08384551	0.01615454	4.60111851
N	−2.71245142	−0.05092517	2.99384935
H	−1.75407039	0.06778769	0.43728135
O	−3.87058573	−0.05439005	0.98588356
C	−1.37264133	−0.03508765	2.55714239
C	−0.37763326	−0.07933045	3.55158864
C	0.96928060	−0.05501425	3.19958259

C	1.35833484	0.00882261	1.85643755
C	0.36471005	0.05326194	0.87861050
C	−0.99536273	0.03091896	1.20684266
H	−0.65730748	−0.12500428	4.60111154
C	2.02883209	−0.15243383	4.27524897
H	2.40689842	0.03254174	1.58421242
C	0.74021692	0.09546940	−0.58931141
C	−6.36850629	−0.07378239	2.55715217
C	−6.74577969	−0.13977682	1.20685047
C	−8.10585113	−0.16208237	0.87861215
C	−9.09947909	−0.11761156	1.85643518
C	−8.71042985	−0.05379557	3.19958244
C	−7.36351661	−0.02951358	3.55159450
H	−5.98706928	−0.17665949	0.43729241
C	−8.48135725	−0.20427220	−0.58931047
H	−10.14804208	−0.14130670	1.58420545
C	−9.76998261	0.04364244	4.27524590
F	−8.23197040	0.99907815	−1.20246027
F	−9.80521896	−0.48331499	−0.78223902
F	−7.76399291	−1.14991243	−1.27180673
F	2.06409064	0.37445564	−0.78223658
F	0.49077093	−1.10785260	−1.20249237
F	0.02289499	1.04116157	−1.27178130
F	2.46342571	−1.44668108	4.43504354
F	1.56918004	0.26115444	5.49837360
F	3.13140939	0.59993293	3.98113082
F	−10.20452704	1.33790309	4.43506451
F	−9.31035161	−0.36998760	5.49836456
F	−10.87258748	−0.70867597	3.98110781

1,3-bis[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −5577.25
H: −5417.16
G: −5466.43
N_{imag} = 0

N	0.93847736	0.78623557	0.05366854
N	−1.14599596	−0.12550294	0.09297390
C	−0.42555439	1.06314000	−0.00589803
C	−2.53879263	−0.31277194	−0.05778750
C	−3.17615049	−1.23352604	0.78296427
C	−4.54334581	−1.48664499	0.63619816
C	−5.28982693	−0.82136343	−0.33717068
C	−4.64079930	0.09169879	−1.17676936
C	−3.27549708	0.34859792	−1.05272510
C	2.01201115	1.70322740	0.11842792
C	3.18343520	1.39702417	−0.58524038
C	4.28862461	2.25013870	−0.51158425
C	4.23697410	3.41743513	0.25121697
C	3.06333097	3.71001123	0.95613408
C	1.95471165	2.86517518	0.90388094
C	2.98887669	4.99199051	1.75936092
H	−2.61223695	−1.74287442	1.56025710
S	−1.09147122	2.57615942	−0.16983756
H	1.20520230	−0.14515707	−0.25446064
H	−2.78743498	1.04689369	−1.71857079
H	−0.67530696	−0.87844747	0.58803689
C	−5.19749390	−2.52827687	1.51657194
H	−6.35141741	−1.01270196	−0.44481742
C	−5.45016235	0.84160305	−2.21439981
H	3.23097228	0.50261579	−1.20124730
C	5.56158107	1.86817614	−1.23393642
H	5.09176922	4.08227503	0.30129666
H	1.06091357	3.09993765	1.46518678

F	−5.02149925	−3.79462249	1.00711358
F	−6.54248353	−2.33508040	1.64221376
F	−4.66633005	−2.54053099	2.78038235
F	−4.68029111	1.28975406	−3.25104498
F	−6.06571313	1.94097452	−1.66880645
F	−6.44021201	0.06192062	−2.75111818
F	4.18587847	5.29186933	2.35412503
F	2.04805439	4.93326704	2.74884305
F	2.66534314	6.06225169	0.96238032
F	6.35318879	2.94672830	−1.50222565
F	5.30744865	1.24074962	−2.42618880
F	6.31702221	0.99382358	−0.48634128

1,3-bis[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −5555.68
H: −5396.00
G: −5446.09
N_{imag} = 0

H	−2.87990544	−0.53380834	3.87180882
H	−4.86120763	0.42483957	3.87193338
N	−5.00376561	0.03385273	2.94342931
C	−3.87060195	−0.05438863	2.15253613
H	−6.91408462	1.60162165	3.85545389
N	−2.73738607	−0.14274743	2.94332983
H	−1.62397666	1.53951365	1.14365294
Se	−3.87069233	−0.05427999	0.32343948
C	−1.38298980	−0.09585568	2.53362231
C	−0.47776281	−0.97774362	3.13243633
C	0.87686436	−0.93178472	2.78382603
C	1.33557131	−0.01893441	1.83425997
C	0.42047579	0.86520118	1.24862005
C	−0.93074875	0.84078372	1.59194071
H	−0.82701660	−1.71034417	3.85545097
C	1.84577035	−1.85810201	3.48410993
H	2.38383718	0.01029557	1.55929775
C	0.90840663	1.83837985	0.19621038
C	−6.35817729	−0.01298364	2.53374037
C	−6.81044796	−0.94967293	1.59213335
C	−8.16167527	−0.97406520	1.24880038
C	−9.07673344	−0.08985688	1.83437729
C	−8.61799494	0.82304247	2.78388854
C	−7.26336659	0.86898592	3.13249060
H	−6.11723902	−1.64846368	1.14390459
C	−8.64954057	−1.94728609	0.19640065
H	−10.12499944	−0.11907146	1.55941787
C	−9.58690478	1.74939009	3.48412668
F	−8.73453355	−1.34932770	−1.03647884
F	−9.89882171	−2.42905382	0.48686551
F	−7.82076492	−3.02552815	0.06016881
F	2.15715830	2.32110344	0.48741826
F	0.99473036	1.24002059	−1.03638144
F	0.07901090	2.91600295	0.05897674
F	1.29803990	−3.09361911	3.71547595
F	2.21419029	−1.35921971	4.71300950
F	2.99419014	−2.04860295	2.77271416
F	−9.03902438	2.98476331	3.71588150
F	−9.95572172	1.25031356	4.71282965
F	−10.73511919	1.94023128	2.77248472

1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]urea

E: −4872.83
H: −4718.98
G: −4761.65

N_{imag} = 0

N	0.94878088	0.77512379	0.19856156
N	−1.14902472	−0.18028393	−0.01199382
C	−0.40696429	1.01428914	0.01098595
C	−2.53572352	−0.33436877	−0.17798355
C	−3.03784690	−1.64976214	−0.19570540
C	−4.40189401	−1.88195216	−0.35664437
C	−5.29897856	−0.81784938	−0.50011633
C	−4.79285436	0.48297647	−0.47873670
C	−3.42788876	0.74231341	−0.32135303
C	2.00746372	1.71366701	0.27604667
C	3.29975120	1.19580362	0.48515626
C	4.39797314	2.05006107	0.57296393
C	4.22542349	3.43382015	0.45357127
C	2.94090967	3.94464878	0.24583287
C	1.82847088	3.10243010	0.15529375
H	2.79259230	5.01810068	0.15135709
H	−2.35925524	−2.49236533	−0.08841498
O	−0.90930265	2.12488258	−0.11950238
H	1.24469345	−0.18868986	0.30524328
H	−3.04973277	1.75509677	−0.30751380
H	−0.64004124	−1.05126048	0.08742821
C	−4.92764141	−3.29928927	−0.31698005
H	−6.35970428	−1.00014021	−0.62535336
C	−5.72741750	1.65793885	−0.68181535
H	3.44161242	0.11931903	0.57910028
H	5.38871210	1.63183680	0.73488476
H	5.08020778	4.10182359	0.52179176
H	0.83716791	3.50387481	−0.00481818
F	−3.98562847	−4.21594455	−0.70763039
F	−6.01704847	−3.47016615	−1.12495454
F	−5.31787412	−3.65636969	0.95303754
F	−5.40229080	2.71984814	0.11698306
F	−7.03150527	1.33813439	−0.41842295
F	−5.68507383	2.11213121	−1.97909383

1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −4790.71
H: −4637.65
G: −4682.92
N_{imag} = 0

C	3.20572336	1.10229703	−1.34744942
C	4.06896578	2.14473195	−1.68860579
C	3.69166459	3.47208689	−1.45959125
C	2.44918877	3.74207593	−0.87544096
C	1.58065457	2.70716291	−0.52149827
C	−1.84718177	−1.68091682	0.27916223
C	−2.20440934	−2.35446644	1.45438732
C	−3.44017886	−3.00277978	1.54540775
C	−4.33742898	−2.97914801	0.47702226
C	−3.96832314	−2.30884260	−0.69572922
C	−2.73531212	−1.66703043	−0.80925695
C	−4.94772239	−2.25015611	−1.84848697
H	3.49525335	0.06978740	−1.53874672
S	−1.31796855	1.23400780	−0.98922810
H	0.08129914	−1.41947165	0.91459114
H	0.62154210	2.92447665	−0.06936373
H	1.66960816	−0.60439991	−0.32464996
H	5.03168930	1.91729318	−2.14010894
H	4.35894685	4.28613783	−1.73126790
H	2.14952351	4.77017363	−0.68578354
H	−1.52621732	−2.36222956	2.30395938

C	−3.77443460	−3.77078360	2.80375765
H	−5.29821862	−3.47531063	0.55131299
H	−2.46052392	−1.16641422	−1.72739103
N	−0.57090998	−1.08593653	0.20994897
N	1.15244414	0.26805277	−0.39520235
C	−0.22300053	0.13408293	−0.38860035
C	1.95642836	1.37781509	−0.76665721
F	−5.84666027	−1.22313861	−1.69185591
F	−5.68345317	−3.40172811	−1.95521736
F	−4.32772530	−2.05440368	−3.05124882
F	−3.30158075	−3.14637602	3.92992777
F	−3.20953303	−5.02673143	2.79059755
F	−5.11827716	−3.94432204	2.97050672

1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −4769.12
H: −4617.05
G: −4661.07
N_{imag} = 0

N	−0.93421772	−0.94004236	−0.07701141
N	−0.78082112	1.31861242	0.10613567
C	−0.06843061	0.14802992	−0.00802232
C	−0.32411876	2.66443785	0.04105116
C	−0.90016956	3.59237521	0.92169365
C	−0.52778612	4.93751847	0.86463218
C	0.42583773	5.36228857	−0.06587011
C	0.99258807	4.43321560	−0.94634731
C	0.62015274	3.08838279	−0.90458766
C	−0.61199681	−2.31416051	−0.02833505
C	−1.29706689	−3.18916790	−0.87808080
C	−1.03703584	−4.56385244	−0.82733729
C	−0.08866173	−5.07568841	0.05758825
C	0.58455482	−4.19106901	0.91061148
C	0.32993797	−2.82057502	0.88212386
C	1.63447039	−4.73825745	1.85299894
H	−1.62978317	3.25713654	1.65725171
Se	1.75809230	0.01498651	−0.06584920
H	−1.84881244	−0.74145388	−0.47557894
H	1.05764596	2.37254622	−1.58967007
H	−1.72175873	1.22099676	0.48102364
H	−0.97724082	5.64829524	1.55390639
H	0.72283178	6.40728072	−0.10676708
H	1.72812422	4.75653591	−1.67917990
H	−2.02022464	−2.80074022	−1.59077670
C	−1.83101282	−5.48931451	−1.72005693
H	0.11803219	−6.13924712	0.09048354
H	0.84548306	−2.15128760	1.55707853
F	−3.09013540	−5.71992718	−1.21125206
F	−1.23754121	−6.70852497	−1.87434154
F	2.83674917	−4.92118849	1.21399316
F	1.27527106	−5.95814248	2.36633285
F	1.87017522	−3.90789349	2.91281758
F	−2.01296275	−4.96292502	−2.97414891

1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]urea

E: −5385.07
H: −5188.34
G: −5230.67
N_{imag} = 0

H	2.79301723	4.02400729	3.27992051
H	2.52200984	4.48625847	1.60129327
H	4.60575635	2.46075499	2.59993117

H	4.94729079	4.06999966	1.96314419
N	0.95722491	0.78157240	0.47002487
N	−1.14369096	−0.18325633	0.23365146
C	−0.38435422	1.00243669	0.22459701
C	−2.52410119	−0.32931325	0.03305828
C	−3.03876602	−1.63966958	−0.00059372
C	−4.40253833	−1.85829245	−0.18510092
C	−5.28783751	−0.78580701	−0.33699405
C	−4.76955035	0.51050641	−0.30042777
C	−3.40531836	0.75610888	−0.12035935
C	−5.69061648	1.69355520	−0.51404044
F	−4.00825465	−4.19093714	−0.56947612
F	−5.64058173	2.14030470	−1.81391513
F	−5.35868923	2.75782370	0.27941409
F	−6.99967073	1.38906574	−0.25329115
F	−6.03698308	−3.42431167	−0.96105617
F	−5.32290966	−3.64305076	1.10881148
H	−2.36949211	−2.48875786	0.11384650
O	−0.86004112	2.11158928	−0.00856849
H	1.23315663	−0.09505015	0.90156192
H	−3.01489539	1.76449443	−0.10158670
H	−0.63010732	−1.05420692	0.30945727
C	−4.93961613	−3.27111899	−0.15999093
H	−6.34791455	−0.95770699	−0.48045292
C	1.88676232	1.90943849	0.64846707
C	4.31685104	2.62956628	0.45744032
C	3.31459876	1.47170076	0.27925109
C	1.82881208	2.49006692	2.07749953
C	2.82772843	3.65086805	2.24868758
C	4.25981047	3.21860798	1.88024404
H	1.55299055	2.68206155	−0.05354284
H	4.08259607	3.42003906	−0.27103170
H	5.33122337	2.28021498	0.22729381
H	3.61198929	0.63282015	0.92990970
H	3.32915584	1.10057604	−0.75301203
H	2.07067446	1.68797072	2.79272088
H	0.80607947	2.82190489	2.28900910

1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −5305.03
H: −5109.64
G: −5152.67
N_{imag} = 0

H	3.28519007	3.18398971	3.78743646
H	2.68294425	4.18500362	2.46808693
H	4.89043598	2.05729855	2.25640279
H	5.12418121	3.80367035	2.17057879
N	0.85523317	1.03425692	0.44915201
N	−1.15175394	−0.03056140	0.18316524
C	−0.50067087	1.17770528	0.46050713
C	−2.53019165	−0.26562597	0.01461241
C	−3.05640911	−1.47624561	0.48653488
C	−4.40847409	−1.77823263	0.29863768
C	−5.25630608	−0.87828588	−0.34862507
C	−4.72030710	0.32506110	−0.82292738
C	−3.37110931	0.63850554	−0.65666271
C	−5.63813106	1.32145589	−1.49781802
F	−4.67417053	−4.10807392	−0.15353528
F	−4.96765079	2.16520487	−2.33882403
F	−6.28818178	2.10933573	−0.57841304
F	−6.61178942	0.70199913	−2.23876676
F	−6.28354108	−3.10882230	0.96821889
F	−4.34874215	−3.51813785	1.94125390

H	−2.41498899	−2.17795821	1.01393816
S	−1.28212589	2.62233831	0.79233047
H	1.24522860	0.14762672	0.14219611
H	−2.97094059	1.56692291	−1.03937948
H	−0.61546269	−0.86849054	0.39053658
C	−4.93303378	−3.11593182	0.76652651
H	−6.30620392	−1.10928555	−0.48686476
C	1.82142306	2.07929229	0.81843231
C	4.17243723	2.94437720	0.41245072
C	3.13154970	1.86945579	0.04031494
C	2.06771866	2.11251816	2.34085913
C	3.10051081	3.19543646	2.70605588
C	4.41839819	2.99770181	1.93283814
H	1.36840318	3.03221317	0.51941113
H	3.81046539	3.92468551	0.06930928
H	5.11081301	2.75012093	−0.12182038
H	3.53916039	0.87340595	0.28012005
H	2.92774660	1.88801313	−1.03805373
H	2.43562193	1.12535873	2.66001472
H	1.11548939	2.29200874	2.85175755

1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −5284.08
H: −5089.04
G: −5132.76
N_{imag} = 0

H	3.33332587	3.11201664	3.81674143
H	2.68134005	4.14729122	2.54827054
H	4.92291348	2.07183540	2.20985010
H	5.12207718	3.82433600	2.18184513
N	0.86328861	1.04102158	0.45961523
N	−1.12988826	−0.04468936	0.19816693
C	−0.48791444	1.15507320	0.48268555
C	−2.50996900	−0.28388986	0.02409942
C	−3.04854183	−1.46791491	0.54117743
C	−4.40336278	−1.76447456	0.35343288
C	−5.23486872	−0.88347685	−0.33815077
C	−4.68331389	0.29348789	−0.86031406
C	−3.33260253	0.59947161	−0.69426322
C	−5.58545032	1.26585919	−1.58827162
F	−4.65743566	−4.11503675	0.01736779
F	−4.89572686	2.08417476	−2.43857665
F	−6.26002764	2.08011454	−0.71082558
F	−6.53944154	0.62027529	−2.33324853
F	−6.30054052	−3.05839951	1.03306027
F	−4.39750030	−3.41392366	2.08674633
H	−2.41833836	−2.15066209	1.10549053
Se	−1.36575627	2.72712814	0.89004922
H	1.26684883	0.15767210	0.15619378
H	−2.91637057	1.50408930	−1.11559303
H	−0.58552467	−0.88606504	0.37244613
C	−4.94464203	−3.07517521	0.87457279
H	−6.28602358	−1.10951933	−0.47581127
C	1.82271506	2.08817761	0.84446051
C	4.14578136	3.01015106	0.41585829
C	3.11646699	1.92925714	0.02854573
C	2.10210620	2.06986068	2.36075679
C	3.12323691	3.15853686	2.74098309
C	4.42602022	3.01384848	1.93124170
H	1.34381120	3.04155851	0.59066203
H	3.75739241	3.99468651	0.11669625
H	5.07478888	2.85339389	−0.14628734
H	3.54779677	0.93305730	0.22215893

H	2.88630355	1.98299475	−1.04323220
H	2.49478640	1.07916595	2.63688954
H	1.15793139	2.21448173	2.89718343

5,6-dihydroindolo[2,3-*b*]indole (X = C; R = 3-CF_3-phenyl)

E: −4738.32
H: −4597.40
G: −4637.56
N_{imag} = 0

C	0.00000000	−0.00000000	−0.07955100
C	−0.02751736	−1.38155841	0.32591486
C	0.02751736	1.38155841	0.32591486
C	−0.00000000	−0.00000000	−1.48034639
C	−0.03888366	−2.06177578	1.55456623
C	−0.04200278	−2.15965596	−0.88505787
C	0.03888366	2.06177578	1.55456623
C	0.04200278	2.15965596	−0.88505787
N	0.02246621	1.27641814	−1.98830637
N	−0.02246621	−1.27641814	−1.98830637
C	−0.06342945	−3.45488796	1.56635814
H	−0.02645621	−1.50894141	2.48994659
C	−0.06652871	−3.54786224	−0.88190300
C	0.06342945	3.45488796	1.56635814
H	0.02645621	1.50894141	2.48994659
C	0.06652871	3.54786224	−0.88190300
H	0.03585183	1.55394994	−2.96000200
H	−0.03585183	−1.55394994	−2.96000200
C	−0.07425440	−4.19153230	0.36373189
H	−0.06887410	−3.98638234	2.51328339
H	−0.07397931	−4.12205678	−1.80343861
C	0.07425440	4.19153230	0.36373189
H	0.06887410	3.98638234	2.51328339
H	0.07397931	4.12205678	−1.80343861
C	−0.14882287	−5.69287512	0.42915474
C	0.14882287	5.69287512	0.42915474
F	0.66776925	−6.21575918	1.40144199
F	0.20380809	−6.29360680	−0.75358080
F	−1.42238903	−6.13764190	0.72329386
F	−0.66776925	6.21575918	1.40144199
F	−0.20380809	6.29360680	−0.75358080
F	1.42238903	6.13764190	0.72329386

5,6-dihydroindolo[2,3-*b*]indole (X = Si; R = 3-CF_3-phenyl)

E: −4617.19
H: −4479.29
G: −4520.44
N_{imag} = 0

Si	−0.05579678	0.92510223	−1.18028164
C	0.35358305	−0.87767080	−0.93475243
C	0.07453290	1.01782643	0.72883939
C	−1.48968098	0.25552965	−2.26013252
N	−0.19545604	−1.72541750	−1.83863221
N	0.90474110	−1.18926950	0.26369736
C	−0.09180429	2.08003091	1.63279055
C	0.79332917	−0.12816356	1.20456894
C	−2.50657746	0.90322601	−2.98090347
C	−1.20825336	−1.10363668	−2.62043546
H	−0.09506952	−2.73726197	−1.83398135
H	1.16216571	−2.12458662	0.56838760
C	0.37994346	2.00078138	2.94372839
C	1.58059361	0.78779814	4.79179044
C	1.32491897	−0.19840754	2.49152573

C	−3.23680820	0.23807273	−3.96668388
C	−3.72933553	−1.80028404	−5.35635782
C	−1.88588331	−1.76323912	−3.64487459
C	1.09784189	0.86898425	3.36630423
H	0.20711085	2.81850216	3.63732922
F	2.05591591	1.98897610	5.25081679
F	2.58535507	−0.13128554	4.95835754
F	0.56981877	0.41821980	5.65446534
H	1.89527563	−1.06454554	2.81636579
C	−2.91685701	−1.08763814	−4.30579790
H	−4.04433882	0.74647889	−4.48536840
F	−4.04778373	−0.98509270	−6.41155533
F	−3.08155096	−2.89286149	−5.87473249
F	−4.92672398	−2.26264492	−4.85144468
H	−1.62974838	−2.78251470	−3.92144704
H	−2.74085848	1.94306752	−2.76295133
H	−0.60771970	2.98258923	1.31204331

5,6-dihydroindolo[2,3-*b*]indole (X = Ge; 3-CF_3-phenyl)

E: −4587.14
H: −4449.76
G: −4491.98
N_{imag} = 0

Ge	0.88365101	1.42536351	−0.00000000
C	1.19094448	−0.56592563	−0.00000000
C	0.03463634	0.88073924	1.79337044
C	0.03463634	0.88073924	−1.79337044
N	1.15064865	−1.17306491	−1.19771632
N	1.15064865	−1.17306491	1.19771632
C	−0.57328665	1.68213558	2.76693305
C	0.55874242	−0.37062960	2.22434508
C	−0.57328665	1.68213558	−2.76693305
C	0.55874242	−0.37062960	−2.22434508
H	1.20626763	−2.18266066	−1.32997925
H	1.20626763	−2.18266066	1.32997925
C	−0.71962349	1.24136904	4.08693195
H	−0.95936696	2.66266574	2.49497045
C	0.47548997	−0.80789496	3.54503563
C	−0.71962349	1.24136904	−4.08693195
H	−0.95936696	2.66266574	−2.49497045
C	0.47548997	−0.80789496	−3.54503563
C	−0.18610624	0.00400095	4.47498838
H	−1.23551039	1.85879215	4.81648324
H	0.91088925	−1.75496768	3.85361483
C	−0.18610624	0.00400095	−4.47498838
H	−1.23551039	1.85879215	−4.81648324
H	0.91088925	−1.75496768	−3.85361483
C	−0.37041717	−0.48579765	5.88883190
C	−0.37041717	−0.48579765	−5.88883190
F	−0.39573246	0.53594666	6.79967627
F	0.62366385	−1.34846409	6.27915165
F	−1.55759249	−1.17188875	6.04146528
F	−0.39573246	0.53594666	−6.79967627
F	0.62366385	−1.34846409	−6.27915165
F	−1.55759249	−1.17188875	−6.04146528

1,3-bis[4-(trifluoromethyl)phenyl]urea

E: −4875.34
H: −4722.00
G: −4762.80
N_{imag} = 0

C	0.06319095	−8.41952394	0.82605314
C	0.07750647	−8.81355901	−0.52448146
C	0.05724666	−9.40701837	1.83193078
N	0.05759936	−7.07599571	1.25009783
C	0.08457797	−10.17099274	−0.84414501
H	0.08422109	−8.06252826	−1.30214477
C	0.06463906	−10.75705567	1.50205985
H	0.04905076	−9.11132823	2.88016332
C	0.05512759	−5.91864109	0.46493062
H	0.04907232	−6.95892232	2.25717363
C	0.08142818	−11.14921848	0.15657761
H	0.09885138	−10.46741547	−1.88877466
H	0.06378049	−11.50536538	2.28887011
N	0.05270534	−4.76128890	1.25010164
O	0.05508915	−5.91863945	−0.76021634
C	0.03648224	−12.61057646	−0.20173425
C	0.04708177	−3.41775908	0.82606224
H	0.06129701	−4.87836572	2.25717649
F	−1.25764355	−13.08505279	−0.26921026
F	0.68288719	−13.39405877	0.72171047
F	0.60646159	−12.87074739	−1.41989997
C	0.03267459	−3.02371825	−0.52446957
C	0.05308884	−2.43026876	1.83194382
C	0.02557565	−1.66628297	−0.84412696
H	0.02591162	−3.77474558	−1.30213573
C	0.04566788	−1.08023033	1.50207913
H	0.06135560	−2.72596342	2.88017455
C	0.02878672	−0.68806173	0.15659949
H	0.01123129	−1.36985583	−1.88875429
H	0.04657463	−0.33192395	2.28889262
C	0.07369993	0.77329911	−0.20170479
F	−0.49631187	1.03346906	−1.41985498
F	1.36781619	1.24779778	−0.26920619
F	−0.57269683	1.55676446	0.72176078

Data S7. Cartesian coordinates and energies of optimized hydrogen-bonded complexes

Below is a list consisting of the Cartesian coordinates (in Å), ADF total bond energies *E*, enthalpies *H*, Gibbs free energies *G* (in kcal mol^{-1}), and the number of imaginary frequencies (N_{imag}) of all optimized hydrogen-bonded complexes reported in this work, optimized at the ZORA-BLYP-D3(BJ)/TZ2P level. It is specified if C_{2v} symmetry is enforced during the optimization process.

Formaldehyde–Urea

E: −1559.34
H: −1497.47
G: −1526.53
N_{imag} = 0

N	1.15351322	−0.46839336	−0.26503547
N	−1.11817925	−0.45487371	0.28420239
C	0.02345509	0.29150225	0.01513160
C	−0.01607548	−4.58541910	−0.03744995
O	0.03297064	1.52266954	0.02409967
O	−0.00672882	−3.37089887	−0.01746189
H	2.02675962	0.04007522	−0.20852825
H	−1.98347145	0.06780697	0.23573500
H	1.17200607	−1.45268468	−0.01961169
H	−1.15188645	−1.43512230	0.02463312
H	0.91469765	−5.17859775	0.09080988
H	−0.95583087	−5.15967113	−0.18493820

Formaldehyde–Thiourea

E: −1481.96
H: −1421.26
G: −1451.64
N_{imag} = 0

N	1.15772326	−0.45957692	−0.16373446
N	−1.12307039	−0.44644661	0.17045731
C	0.02337417	0.27975018	0.01617927
C	−0.01570226	−4.54440136	−0.03253933
S	0.03733297	1.96458766	0.04532135
O	−0.00622696	−3.32843844	−0.03157409
H	2.03428966	0.04094910	−0.18879618
H	−1.99126107	0.06716077	0.21457674
H	1.15630215	−1.47085856	−0.07861506
H	−1.13802496	−1.45443015	0.05371417
H	0.92507071	−5.13397724	−0.01748645
H	−0.96557504	−5.11919043	−0.04854847

Formaldehyde–Selenourea

E: −1461.19
H: −1400.77
G: −1431.77
N_{imag} = 0

N	1.16464857	−0.46852983	−0.09231803
N	−1.13005006	−0.45253332	0.10541604
C	0.02289441	0.25660871	0.01352752
C	−0.01540095	−4.53117682	−0.03391233
Se	0.03733358	2.11052964	0.03153876
O	−0.00602287	−3.31424834	−0.02229106
H	2.03575099	0.03697806	−0.16322662
H	−1.99317705	0.06507003	0.18594170

H	1.16116448	−1.48408686	−0.10403711
H	−1.14245493	−1.46805454	0.09669327
H	0.92177961	−5.11917779	−0.12329958
H	−0.96155915	−5.10625402	0.04433119

Formaldehyde–1-cyclohexylurea

E: −3583.20
H: −3426.89
G: −3461.73
N_{imag} = 0

N	3.27482333	−0.24713294	−5.96070818
N	1.00213148	0.08412114	−6.38481949
C	2.18080458	0.58327307	−5.81938038
C	2.27266307	−3.87998088	−7.73137135
H	5.71934466	−0.75223811	−2.01719951
O	2.13733361	−2.69017478	−7.52843861
H	1.58186334	−4.44021423	−8.39727135
O	2.21611645	1.66759189	−5.23007485
H	5.92020322	0.76336012	−2.89424330
H	6.88464303	−1.99997021	−3.82802307
H	3.09314885	−4.46401142	−7.26113074
H	0.29535906	0.79496973	−6.53282633
H	3.11756372	−1.18297723	−6.32478091
H	1.06982199	−0.62769185	−7.10549715
H	7.91247784	−0.68022269	−3.26596604
C	4.51378207	−0.00508877	−5.21880574
C	7.03569934	−0.35560261	−5.23339538
C	5.71216977	−0.58953550	−5.98802083
C	4.45374552	−0.56272365	−3.77886552
C	5.77496628	−0.31961921	−3.02462236
C	6.97589814	−0.90299062	−3.79387071
H	4.62252362	1.08449405	−5.15784701
H	7.24093968	0.72491915	−5.19925534
H	7.86658399	−0.81624176	−5.78371423
H	5.55745346	−1.67323427	−6.12059326
H	5.75293889	−0.14639874	−6.99098823
H	4.25148377	−1.64449965	−3.82988197
H	3.61235038	−0.09724504	−3.25312635

Formaldehyde–1-cyclohexylthiourea

E: −3506.80
H: −3351.02
G: −3388.31
N_{imag} = 0

H	0.66238050	−0.37001684	1.34224472
H	−1.35148484	−0.74811382	0.51622071
N	−1.20588488	−0.01474794	−0.17137512
C	0.06125029	0.46180403	−0.42409573
S	0.38553010	1.38076091	−1.80468772
N	0.98278057	0.14619259	0.52557667
C	2.47131995	2.01006121	1.24543394
C	3.93128694	2.49912130	1.28266667
C	4.85441343	1.46219604	1.95125242
C	4.73703480	0.08622015	1.26680895
C	3.27617354	−0.40369011	1.21798475
H	5.89657971	1.80654858	1.92754725
H	2.65882063	0.76204974	−0.50103213
H	1.83195579	2.72451457	0.71555084
H	2.08478157	1.91596838	2.27236770
H	−1.85849634	0.05138160	−0.94101765
H	4.57756800	1.36274167	3.01249172
H	3.20523218	−1.35606148	0.67700096

C	2.36251623	0.63765668	0.54766722
H	2.92076799	−0.58608278	2.24596030
H	4.27476746	2.68104385	0.25339470
H	3.99191052	3.46048364	1.80877650
H	5.36158289	−0.65374712	1.78408761
H	5.12189593	0.16082607	0.23894538
H	0.44638395	−2.46780698	4.02356338
O	−0.56240523	−1.73911754	2.41699891
H	−1.24694847	−3.21416023	3.63384333
C	−0.45265356	−2.48394388	3.37135742

Formaldehyde–1-cyclohexylselenourea

E: −3486.50
H: −3331.04
G: −3369.27
N_{imag} = 0

N	3.22209046	−0.27532978	−5.83276676
N	1.03309910	0.08212880	−6.44011295
C	2.15895956	0.56025573	−5.83348804
C	2.33284166	−3.79616462	−7.87356063
H	5.80028545	−0.62000488	−1.97292194
O	2.14590732	−2.67837613	−7.43135050
H	1.59963130	−4.28420256	−8.54922572
Se	2.15363898	2.25604572	−5.06643743
H	5.99486244	0.84143556	−2.93905977
H	6.87287102	−1.98881203	−3.75350775
H	3.24456583	−4.37763227	−7.62126580
H	0.26663379	0.73102458	−6.55314062
H	3.09765652	−1.19945014	−6.24382862
H	1.04827394	−0.77097922	−6.99149135
H	7.94588940	−0.66202735	−3.30400443
C	4.49826906	−0.01859275	−5.15730982
C	7.00261408	−0.42677200	−5.25210862
C	5.64709673	−0.67270682	−5.94414319
C	4.47304061	−0.50021654	−3.69210011
C	5.82654716	−0.24379492	−3.00362493
C	6.98586024	−0.89374950	−3.78338488
H	4.62643489	1.07087410	−5.15861277
H	7.22905875	0.64914431	−5.28591126
H	7.80195347	−0.93483644	−5.80700485
H	5.46635308	−1.75845185	−6.01256657
H	5.65934605	−0.28100786	−6.96929198
H	4.24602308	−1.57782222	−3.67607883
H	3.66239693	0.01773289	−3.16773697

Formaldehyde–1-phenylurea

Global minimum
E: −3073.92
H: −2959.79
G: −2995.21
N_{imag} = 0

N	−0.98946711	0.03556856	0.53508894
N	−3.27370354	−0.34877490	0.54483561
C	−2.24647496	0.52538037	0.18738715
C	−0.61353805	−2.99992311	−0.68792553
O	−2.45939827	1.61769026	−0.33493422
O	−1.24287763	−2.98369736	0.35447337
H	−0.41516285	−3.95017121	−1.22698175
H	−4.17300308	−0.10887960	0.14525651
H	−0.97752976	−0.89009652	0.95531548
H	−3.07646865	−1.33987396	0.64133325

H	−0.21133362	−2.06998567	−1.14126449
H	−0.39271575	2.40341245	−0.68066399
C	0.27698701	0.59542113	0.28122147
C	1.40171428	−0.14573803	0.70022815
C	2.69194562	0.33192331	0.47009510
C	2.88654271	1.55623655	−0.17957914
C	1.76983197	2.29280237	−0.58909832
C	0.46986627	1.83007269	−0.36678997
H	1.25690876	−1.09185550	1.22015732
H	3.54576158	−0.25332777	0.80489171
H	3.89125614	1.93123779	−0.35786650
H	1.90626480	3.24886045	−1.09041854

Local minimum
E: −3073.52
H: −2960.01
G: −2994.31
N_{imag} = 0

N	−0.97041216	0.09619172	0.12687970
N	−3.25826861	−0.25778940	0.27610916
C	−2.23471989	0.67951603	0.13404334
C	−0.63500407	−3.83553764	−0.08988807
O	−2.45695417	1.88745561	0.06720745
O	−1.42916602	−2.91852977	−0.01233618
H	−0.96947336	−4.88049904	−0.25783244
H	−4.17976135	0.10623133	0.06746270
H	−0.94600859	−0.91966110	0.18020973
H	−3.09419817	−1.23206819	0.04657623
H	0.45970547	−3.67001420	0.00343008
H	−0.41050618	2.75976788	−0.06341879
C	0.28558423	0.72414690	0.04366493
C	1.42373220	−0.10887885	0.05941541
C	2.70560063	0.43368641	−0.02120020
C	2.88085639	1.81909764	−0.11868306
C	1.75235562	2.64555783	−0.13293085
C	0.46063667	2.11781975	−0.05313874
H	1.29489742	−1.18773636	0.13893176
H	3.56905383	−0.22821853	−0.00630934
H	3.87921306	2.24495302	−0.18109108
H	1.87283706	3.72450898	−0.20710173

Formaldehyde–1-phenylthiourea

E: −2994.31
H: −2881.33
G: −2917.71
N_{imag} = 0

N	−1.01128868	0.10055562	0.52661417
N	−3.22648151	−0.44356180	0.59205885
C	−2.28652408	0.47919240	0.17446365
C	−0.63612808	−2.88697388	−0.75010821
S	−2.76280592	1.88132561	−0.61674107
O	−1.17688789	−2.92594249	0.34071381
H	−0.40076613	−3.81615865	−1.30989554
H	−4.16623336	−0.27849837	0.25420650
H	−0.96570787	−0.79919114	1.00176453
H	−2.95214524	−1.41055242	0.74752709
H	−0.35614570	−1.92574457	−1.22863500
H	−0.32432507	2.43463731	−0.77104751
C	0.26670792	0.64053417	0.26514767
C	1.36056098	−0.11849592	0.73509313
C	2.66865697	0.31227582	0.52196247
C	2.91380322	1.50803857	−0.16385797

C	1.82973082	2.26111543	−0.62421171
C	0.51103600	1.84444482	−0.41750371
H	1.17626203	−1.04443942	1.27836242
H	3.49619665	−0.28633499	0.89615679
H	3.93300122	1.84782075	−0.33028027
H	2.00469822	3.19550773	−1.15330382

Formaldehyde–1-phenylselenourea

E: −2973.04
H: −2861.02
G: −2896.77
N_{imag} = 0

N	−0.99956755	0.05284079	0.37954009
N	−3.22071242	−0.46572825	0.40411813
C	−2.27330779	0.49921734	0.16922890
C	−0.63440783	−3.04021609	−0.74398404
Se	−2.83419999	2.17329930	−0.38212261
O	−1.00525354	−2.93394302	0.41146438
H	−0.50798139	−4.03458262	−1.21938668
H	−4.18316252	−0.15368839	0.41064737
H	−0.94224886	−0.91172649	0.71444150
H	−2.99153429	−1.33047337	0.88642694
H	−0.40824423	−2.14996190	−1.36733862
H	−0.31393785	2.40460354	−0.88051153
C	0.27677488	0.63576492	0.19777805
C	1.36415280	−0.09337823	0.72291243
C	2.66888094	0.37386975	0.57288687
C	2.91335921	1.57685118	−0.10051848
C	1.83378673	2.29727804	−0.62012810
C	0.51977043	1.84028439	−0.48142827
H	1.17750398	−1.02248518	1.25911240
H	3.49364706	−0.20008595	0.98937080
H	3.92954391	1.94616912	−0.21482555
H	2.00886522	3.23331105	−1.14626149

Formaldehyde–1-[3-(trifluoromethyl)phenyl]urea

E: −3469.63
H: −3351.95
G: −3390.27
N_{imag} = 0

N	−0.98280576	0.23205759	0.24931064
N	−3.16734823	−0.39925818	0.69137348
C	−2.27820743	0.65981892	0.54267842
C	−0.14688563	−3.43446941	−0.80369116
O	−2.61342545	1.83236312	0.69774919
O	−1.02229814	−2.72485604	−0.34455027
H	−0.35257442	−4.48096718	−1.10964444
H	−4.14289122	−0.12985193	0.70937194
H	−0.85380684	−0.77184080	0.13236095
H	−2.95080804	−1.31464032	0.31246616
H	0.89330988	−3.06975842	−0.93804959
H	1.34954795	−0.76557048	−0.30211745
C	0.16636071	1.00959605	0.05117765
C	0.19433450	2.41602607	0.12766566
C	1.39427610	3.09406690	−0.09869383
C	2.57624379	2.41355612	−0.40075247
C	2.54369738	1.01468444	−0.47411474
C	1.35688219	0.31889942	−0.24660737
H	−0.71850341	2.94945252	0.35890373
H	1.40281335	4.17995904	−0.03978432
H	3.50088452	2.95272662	−0.58015376

C	3.81239372	0.24548160	−0.74206202
F	4.65400734	0.90068494	−1.60014128
F	3.57210564	−0.99545422	−1.29045488
F	4.53210994	0.01887136	0.41110628

Formaldehyde–1-[3-(trifluoromethyl)phenyl]thiourea

E: −3389.73
H: −3273.22
G: −3312.34
N_{imag} = 0

N	−0.94336428	0.22638416	0.23484750
N	−3.09811587	−0.39436637	0.65344835
C	−2.21668862	0.65546620	0.54123713
C	−0.28752804	−3.47191346	−0.92779589
S	−2.73407419	2.23132120	0.80591558
O	−1.07738698	−2.72578157	−0.37846951
H	−0.58702577	−4.48849115	−1.25517034
H	−4.07187733	−0.14945056	0.77051820
H	−0.85218776	−0.78454500	0.12589352
H	−2.86807388	−1.32679091	0.32441057
H	0.76222950	−3.17027151	−1.12547924
H	−0.41871699	2.93930701	0.19117969
C	0.26786976	0.90532526	0.01354409
C	1.38686495	0.08341542	−0.22798123
C	2.63652629	0.64008609	−0.49043141
C	2.80716698	2.03139847	−0.50478477
C	1.69824116	2.84174878	−0.25584171
C	0.43502644	2.30163726	0.00109938
H	1.27283707	−0.99598315	−0.20875709
C	3.82194723	−0.26718859	−0.70301464
H	3.78099234	2.46450161	−0.71023623
F	4.52612096	−0.47909102	0.46097359
F	4.71405243	0.23862043	−1.60920109
F	3.45526839	−1.51528693	−1.15969825
H	1.81284530	3.92308213	−0.26504701

Formaldehyde–1-[3-(trifluoromethyl)phenyl]selenourea

E: −3368.51
H: −3252.95
G: −3291.38
N_{imag} = 0

N	−0.96629331	0.24241420	0.12693599
N	−3.16341246	−0.34225368	0.24253217
C	−2.26258617	0.68181690	0.18568985
C	−0.15937843	−3.56675657	−0.34429664
Se	−2.88606305	2.42358160	0.21443550
O	−1.01944704	−2.76566427	−0.02526532
H	−0.40243813	−4.63517535	−0.51538437
H	−4.14252402	−0.09647515	0.28831598
H	−0.86381839	−0.77437594	0.15223083
H	−2.89154790	−1.31993477	0.21039599
H	0.90032233	−3.26514013	−0.47771729
H	−0.41467618	2.92467315	−0.23338166
C	0.27435575	0.90159405	0.03188616
C	1.40804804	0.07105334	0.12486537
C	2.69062586	0.60311380	0.01038389
C	2.87502988	1.97911237	−0.18377260
C	1.74827075	2.79879198	−0.26742382
C	0.45416624	2.28113793	−0.16556901
H	1.28071344	−0.99447190	0.28935944
C	3.88524402	−0.30549746	0.15462194
H	3.87454643	2.39290679	−0.27291302

F	4.36256693	−0.33136584	1.44561247
F	4.93294767	0.07562765	−0.63886424
F	3.59423511	−1.61321630	−0.17107076
H	1.87387712	3.86781411	−0.42194160

Formaldehyde–1-[3,5-bis(trifluoromethyl)phenyl]urea

E: −3863.05
H: −3741.30
G: −3784.01
N_{imag} = 0

N	−0.97865241	0.12952767	0.03490702
N	−3.23617740	−0.37668520	−0.08534019
C	−2.27220850	0.61413700	−0.19128587
C	−0.27469045	−3.74323726	0.29661636
O	−2.54539534	1.78922533	−0.42219710
O	−1.11242036	−2.86402552	0.21779704
H	−0.55386721	−4.81478764	0.23205209
H	−4.15800324	−0.11343544	−0.40927532
H	−0.89058879	−0.87234729	0.19918796
H	−2.98840495	−1.35873536	−0.12774571
H	0.80289592	−3.51433710	0.43569218
H	−0.59059356	2.79700717	−0.37811427
C	0.22268913	0.84340967	0.02587821
C	1.40389549	0.11180606	0.26058567
C	2.64349387	0.74631178	0.25910305
C	2.74441115	2.12340134	0.03163558
C	1.56896849	2.84406539	−0.19385940
C	0.31338330	2.22912284	−0.20177312
H	1.34627911	−0.95738709	0.44153816
C	3.88813935	−0.05216293	0.56621352
H	3.70888825	2.61722398	0.03122475
C	1.64715401	4.32617816	−0.49543749
F	2.80836181	4.89081471	−0.03827116
F	0.61261403	5.02486289	0.06219575
F	1.60027104	4.56508995	−1.84988841
F	4.98148076	0.40103074	−0.11749566
F	3.74415446	−1.38478206	0.25651459
F	4.21019671	−0.00007429	1.90308728

Formaldehyde–1-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −3782.83
H: −3662.28
G: −3705.82
N_{imag} = 0

N	−1.03854796	0.20608217	0.05181554
N	−3.21969139	−0.45721752	−0.01712838
C	−2.35287499	0.60238049	−0.11125092
C	−0.14210512	−3.65482475	0.21676287
S	−2.92572581	2.15816220	−0.36574473
O	−1.00525183	−2.79613712	0.23084602
H	−0.40062915	−4.73119383	0.15235242
H	−4.19412875	−0.26409484	−0.20319190
H	−0.91189981	−0.79525342	0.20562784
H	−2.90346389	−1.42132050	0.00199734
H	0.93713311	−3.40014956	0.26684883
H	−0.56568618	2.88413763	−0.40719436
C	0.17426347	0.90899558	0.03088509
C	1.32980055	0.14035207	0.27982794
C	2.59173024	0.72590964	0.26527637
C	2.74253188	2.09464821	0.01265385
C	1.59412697	2.85210543	−0.22505405
C	0.31596965	2.28358961	−0.22217888

H	1.23250234	−0.92112297	0.48487030
C	3.80627176	−0.11369107	0.58331306
H	3.72440213	2.55331628	0.00278803
C	1.72592376	4.32490644	−0.55559173
F	2.89576714	4.86012630	−0.08495506
F	0.70379393	5.06698214	−0.03542143
F	1.71622748	4.53434851	−1.91537134
F	4.90568848	0.26818585	−0.13272379
F	3.60034422	−1.44955874	0.32217295
F	4.15144776	−0.02943669	1.91166064

Formaldehyde–1-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −3761.56
H: −3641.37
G: −3685.80
N_{imag} = 0

N	−1.04517801	0.18928275	0.09720800
N	−3.23210999	−0.44544651	0.06069290
C	−2.35595956	0.59940690	0.07293091
C	−0.08426563	−3.60350248	−0.08353648
Se	−3.00292862	2.32888063	0.08220039
O	−0.98141561	−2.80110738	0.10359799
H	−0.29558153	−4.68467117	−0.20849460
H	−4.21803332	−0.22464657	0.09062619
H	−0.91405439	−0.82198683	0.17397554
H	−2.93512639	−1.41573541	0.09982132
H	0.97878935	−3.28940222	−0.13736659
H	−0.56546172	2.82672110	−0.52719381
C	0.17091670	0.89124303	0.07156997
C	1.31850012	0.14414752	0.39519326
C	2.58231006	0.73008343	0.35752489
C	2.73423576	2.07682007	0.01371060
C	1.58901544	2.81405665	−0.30146357
C	0.31395788	2.24286431	−0.28407002
H	1.21637633	−0.89786293	0.68347281
C	3.78490975	−0.09252003	0.75476082
H	3.71550553	2.53660970	−0.00942070
C	1.74094076	4.25526704	−0.74328500
F	2.80569117	4.86973434	−0.13676669
F	0.63372991	5.00476730	−0.47618773
F	1.96217678	4.33915447	−2.10005321
F	4.93594229	0.34136089	0.16293476
F	3.63497653	−1.42074160	0.41913662
F	4.00006041	−0.06254946	2.11237398

Formaldehyde–1,3-dicyclohexylurea

E: −5606.83
H: −5353.74
G: −5401.58
N_{imag} = 0

H	−0.05777810	1.09467044	−1.13238953
H	0.05777810	−1.09467044	−1.13238953
N	0.26463644	−1.13583656	−0.13835780
C	−0.00000000	0.00000000	0.61597988
O	−0.00000000	0.00000000	1.85359185
N	−0.26463644	1.13583656	−0.13835780
H	2.17816014	4.80703455	1.40201692
H	0.74561562	4.35425424	2.32397147
H	0.76309224	5.54873471	−0.50629247
H	0.25222783	6.37944570	0.96460919
C	−0.25665674	2.46337665	0.48155254
C	−1.13301874	4.84558631	0.27584117

C	−1.11690114	3.43516896	−0.34590272
C	1.17339261	3.01680103	0.67476917
C	1.15431624	4.42282332	1.30447932
C	0.29235914	5.39617597	0.47753237
H	−0.70958609	2.33719862	1.47217926
H	−1.64241824	4.80069532	1.25026630
H	−1.72011160	5.52610073	−0.35487060
H	−0.70674404	3.49428040	−1.36763972
H	−2.13552232	3.03639839	−0.43198616
H	1.66841728	3.05966900	−0.30855927
H	1.74277541	2.31789502	1.29800555
C	−1.17339261	−3.01680103	0.67476917
C	−1.15431624	−4.42282332	1.30447932
C	0.25665674	−2.46337665	0.48155254
H	−1.74277541	−2.31789502	1.29800555
H	−1.66841728	−3.05966900	−0.30855927
C	−0.29235914	−5.39617597	0.47753237
H	−2.17816014	−4.80703455	1.40201692
H	−0.74561562	−4.35425424	2.32397147
C	1.11690114	−3.43516896	−0.34590272
H	0.70958609	−2.33719862	1.47217926
C	1.13301874	−4.84558631	0.27584117
H	−0.25222783	−6.37944570	0.96460919
H	−0.76309224	−5.54873471	−0.50629247
H	2.13552232	−3.03639839	−0.43198616
H	0.70674404	−3.49428040	−1.36763972
H	1.72011160	−5.52610073	−0.35487060
H	1.64241824	−4.80069532	1.25026630
C	0.00000000	0.00000000	−4.29855089
H	0.08706112	0.94147473	−4.88262234
H	−0.08706112	−0.94147473	−4.88262234
O	0.00000000	0.00000000	−3.08422616

Formaldehyde–1,3-dicyclohexylthiourea

E: −5531.02
H: −5280.22
G: −5324.90
N_{imag} = 0

H	−0.06778414	1.05314379	−1.01341577
H	0.06591666	−1.05336422	−1.01334941
N	0.17041779	−1.13499789	−0.00483617
C	−0.00104085	−0.00006341	0.74210287
S	−0.00116237	−0.00001850	2.43750596
N	−0.17239021	1.13483175	−0.00491800
H	2.15896043	4.92559541	1.37825902
H	0.70842080	4.50097236	2.28540449
H	0.78770776	5.52904054	−0.60915990
H	0.22023066	6.43482594	0.79511822
C	−0.20968316	2.49517064	0.53660689
C	−1.11869875	4.83912817	0.15987156
C	−1.06241366	3.39470273	−0.37586057
C	1.20629534	3.07881850	0.73129450
C	1.14476172	4.51832618	1.27547706
C	0.29128476	5.42565705	0.36844788
H	−0.68635082	2.41921625	1.52103652
H	−1.65568883	4.84235381	1.12009828
H	−1.69803517	5.46976505	−0.52715699
H	−0.62517125	3.40023460	−1.38813718
H	−2.07247717	2.97437849	−0.46298037
H	1.72772790	3.07090198	−0.23890569
H	1.76357402	2.42614060	1.41215680
C	−1.20842796	−3.07892005	0.73124541
C	−1.14701489	−4.51840235	1.27550880

C	0.20759432	−2.49531037	0.53676466
H	−1.76580692	−2.42619786	1.41198338
H	−1.72969995	−3.07104030	−0.23904142
C	−0.29340519	−5.42579488	0.36866651
H	−2.16123922	−4.92564529	1.37814161
H	−0.71084177	−4.50100777	2.28550809
C	1.06046071	−3.39490573	−0.37551343
H	0.68409894	−2.41931249	1.52126971
C	1.11662578	−4.83930616	0.16029970
H	−0.22244498	−6.43494503	0.79539671
H	−0.78966594	−5.52921398	−0.60901987
H	2.07054740	−2.97460592	−0.46248271
H	0.62338973	−3.40047900	−1.38786387
H	1.69606568	−5.46998875	−0.52659956
H	1.65345322	−4.84249536	1.12061755
C	−0.00026440	−0.00015061	−4.14688062
H	0.01992670	0.94521176	−4.72958873
H	−0.02008999	−0.94549871	−4.72962429
O	−0.00065231	−0.00016547	−2.93153970

Formaldehyde–1,3-dicyclohexylselenourea

E: −5511.05
H: −5260.55
G: −5305.91
N_{imag} = 0

H	−0.06871339	1.05614501	−1.01483806
H	0.06783163	−1.05639429	−1.01475180
N	0.14430769	−1.13696759	−0.00258851
C	−0.00124661	−0.00010623	0.73086577
Se	−0.00212658	−0.00009106	2.59901886
N	−0.14610158	1.13673998	−0.00274550
H	2.16159996	4.94364855	1.36689495
H	0.71781840	4.50794741	2.27967258
H	0.77837082	5.53759018	−0.61518379
H	0.20954225	6.43886423	0.79140085
C	−0.19269883	2.49920808	0.53636993
C	−1.12014285	4.83389819	0.16105142
C	−1.05573861	3.38968938	−0.37465012
C	1.22014399	3.09039173	0.72386875
C	1.14995674	4.52928720	1.26811860
C	0.28646213	5.43035176	0.36429132
H	−0.66431734	2.41992138	1.52323191
H	−1.65355282	4.83308634	1.12316681
H	−1.70654167	5.46000084	−0.52403367
H	−0.62287351	3.39764424	−1.38882396
H	−2.06330937	2.96224790	−0.45644070
H	1.73853952	3.08528039	−0.24794070
H	1.78251827	2.44135962	1.40415929
C	−1.22284546	−3.09042883	0.72282141
C	−1.15334350	−4.52932108	1.26716404
C	0.19024504	−2.49943245	0.53659765
H	−1.78575410	−2.44130811	1.40258484
H	−1.74035214	−3.08527067	−0.24946149
C	−0.28915025	−5.43051324	0.36413449
H	−2.16513107	−4.94354601	1.36503196
H	−0.72211863	−4.50801808	2.27910861
C	1.05399776	−3.39004250	−0.37361788
H	0.66097471	−2.42018770	1.52388756
C	1.11771917	−4.83425089	0.16216842
H	−0.21275481	−6.43903184	0.79132394
H	−0.78018243	−5.53769486	−0.61578676
H	2.06170052	−2.96273738	−0.45449556
H	0.62205916	−3.39795891	−1.38818703

H	1.70466104	−5.46044374	−0.52236875
H	1.65024873	−4.83349310	1.12477169
C	0.00106207	0.00007079	−4.12892038
H	0.01802878	0.94550710	−4.71102382
H	−0.01530723	−0.94521687	−4.71128183
O	0.00043713	−0.00008462	−2.91269435

Formaldehyde–1,3-diphenylurea

E: −4587.19
H: −4421.98
G: −4462.30
N_{imag} = 0

N	0.17471484	3.05648197	−0.24606526
N	0.19881751	0.75011517	−0.24606474
C	0.18676841	1.90329876	0.54188283
C	0.21360525	−0.59524717	0.17070599
C	0.22178803	−1.57612818	−0.84293322
C	0.23687596	−2.93217792	−0.52040817
C	0.24404008	−3.33997667	0.81892908
C	0.23587590	−2.36706478	1.82350231
C	0.22073631	−1.00298838	1.51807934
C	0.15992418	4.40184446	0.17070483
C	0.15173956	5.38272495	−0.84293488
C	0.13665113	6.73877486	−0.52041053
C	0.12948292	7.14657426	0.81892650
C	0.13765717	6.17366300	1.82350024
C	0.15279624	4.80958643	1.51807797
H	0.13225072	6.47504649	2.86907306
H	0.21625181	−1.26508438	−1.88698154
O	0.18676854	1.90329900	1.77104729
H	0.17701025	2.92588943	−1.25328404
H	0.21436909	−0.25472174	2.29912835
H	0.19651917	0.88070722	−1.25328355
H	0.24297452	−3.67150334	−1.31862185
H	0.25575652	−4.39701352	1.07292701
H	0.24128030	−2.66844777	2.86907529
H	0.15727364	5.07168062	−1.88698304
H	0.13054910	7.47809983	−1.31862460
H	0.11776120	8.20361119	1.07292387
H	0.15916352	4.06132021	2.29912738
H	0.19505760	0.95761582	−4.91910048
H	0.17848023	2.84899885	−4.91909197
C	0.18676591	1.90330469	−4.33804757
O	0.18676425	1.90329924	−3.12224829

Formaldehyde–1,3-diphenylthiourea

E: −4504.57
H: −4341.86
G: −4379.59
N_{imag} = 0

N	0.14227043	3.03602369	−0.06349009
N	0.23225054	0.77083317	−0.06276762
C	0.18635320	1.90360441	0.73573897
C	0.18692813	−0.60624153	0.24737387
C	0.70448121	−1.48115864	−0.72992234
C	0.66498974	−2.86203967	−0.54246400
C	0.11215257	−3.39828749	0.62648597
C	−0.40641585	−2.53082705	1.59307808
C	−0.37951482	−1.14469714	1.41561533
C	0.18658842	4.41310470	0.24691265
C	−0.33374840	5.28794416	−0.72889427
C	−0.29492150	6.66880764	−0.54092256

C	0.25993534	7.20495967	0.62709668
C	0.78131156	6.33751955	1.59222714
C	0.75517626	4.95147302	1.41413801
H	1.22209644	6.74026321	2.50174522
H	1.14522639	−1.06688752	−1.63577605
S	0.18439365	1.90433157	2.41062578
H	−0.03829490	2.86353674	−1.04997149
H	−0.77927098	−0.48309629	2.17179392
H	0.41369279	0.94313463	−1.04912443
H	1.07368938	−3.51837072	−1.30773950
H	0.08603368	−4.47438719	0.77964223
H	−0.84555288	−2.93358900	2.50338619
H	−0.77619723	4.87367584	−1.63391371
H	−0.70578798	7.32516028	−1.30501680
H	0.28548260	8.28101209	0.78068657
H	1.15722599	4.28988376	2.16912233
H	0.55473489	1.03003938	−4.73463871
H	−0.17624214	2.77465536	−4.73534419
C	0.18897972	1.90247116	−4.15413267
O	0.18842359	1.90273082	−2.93814686

Formaldehyde–1,3-diphenylselenourea

E: −4482.93
H: −4320.06
G: −4360.41
N_{imag} = 0

N	−0.06014730	1.13085606	0.04731188
N	0.06014730	−1.13085606	0.04731188
C	0.00000000	−0.00000000	0.83291408
C	0.00269119	−2.50491123	0.38443809
C	0.71668479	−3.39204335	−0.44167640
C	0.66856104	−4.76801340	−0.21178301
C	−0.08819818	−5.27680461	0.84946115
C	−0.80441031	−4.39320103	1.66475071
C	−0.77131940	−3.01508027	1.43880763
C	−0.00269119	2.50491123	0.38443809
C	−0.71668479	3.39204335	−0.44167640
C	−0.66856104	4.76801340	−0.21178301
C	0.08819818	5.27680461	0.84946115
C	0.80441031	4.39320103	1.66475071
C	0.77131940	3.01508027	1.43880763
H	1.40434869	4.77790751	2.48667062
H	1.31935120	−2.99427400	−1.25681160
Se	0.00000000	−0.00000000	2.67688616
H	−0.27237192	0.96938591	−0.93580373
H	−1.32726699	−2.33689784	2.07298175
H	0.27237192	−0.96938591	−0.93580373
H	1.23123964	−5.43966249	−0.85639729
H	−0.12052806	−6.34734334	1.03715830
H	−1.40434869	−4.77790751	2.48667062
H	−1.31935120	2.99427400	−1.25681160
H	−1.23123964	5.43966249	−0.85639729
H	0.12052806	6.34734334	1.03715830
H	1.32726699	2.33689784	2.07298175
H	0.42550597	−0.84466544	−4.61145154
H	−0.42550597	0.84466544	−4.61145154
C	0.00000000	−0.00000000	−4.03077073
O	0.00000000	−0.00000000	−2.81434258

Formaldehyde–1,3-bis[3-(trifluoromethyl)phenyl]urea

E: −5378.32
H: −5204.75
G: −5252.56

N_{imag} = 0

N	0.00897777	1.15194557	0.23712105
N	−0.00897777	−1.15194557	0.23712105
C	0.00000000	−0.00000000	1.02685307
C	−0.02229998	−2.49333209	0.65611415
C	−0.02502089	−3.47025066	−0.35798771
C	−0.04493502	−4.82587772	−0.03244235
C	−0.05736069	−5.23903916	1.30657467
C	−0.05353113	−4.26557998	2.30731736
C	−0.03586364	−2.90219407	2.00319160
C	0.02229998	2.49333209	0.65611415
C	0.02502089	3.47025066	−0.35798771
C	0.04493502	4.82587772	−0.03244235
C	0.05736069	5.23903916	1.30657467
C	0.05353113	4.26557998	2.30731736
C	0.03586364	2.90219407	2.00319160
F	0.47496786	5.37870915	−2.32830831
H	−0.01822349	−3.16501933	−1.40094739
O	0.00000000	−0.00000000	2.25514199
H	0.00482112	1.02017145	−0.77084542
H	−0.03464821	−2.15467091	2.78499001
H	−0.00482112	−1.02017145	−0.77084542
C	0.00710607	−5.85628083	−1.13340533
H	−0.07544453	−6.29522280	1.55569429
F	0.71549839	6.98013780	−0.83286883
H	0.01822349	3.16501933	−1.40094739
C	−0.00710607	5.85628083	−1.13340533
H	0.07544453	6.29522280	1.55569429
H	0.03464821	2.15467091	2.78499001
F	1.29632919	−6.27756200	−1.37947160
F	−0.47496786	−5.37870915	−2.32830831
F	−0.71549839	−6.98013780	−0.83286883
F	−1.29632919	6.27756200	−1.37947160
H	0.06663936	4.57044849	3.35105584
H	−0.06663936	−4.57044849	3.35105584
H	−0.00609724	−0.94597226	−4.39717925
H	0.00609724	0.94597226	−4.39717925
C	−0.00000000	−0.00000000	−3.81822171
O	−0.00000000	−0.00000000	−2.60097896

Formaldehyde–1,3-bis[3-(trifluoromethyl)phenyl]thiourea

E: −5295.39
H: −5123.61
G: −5170.58
N_{imag} = 0

N	−0.94076821	0.61734903	0.55031729
N	1.22600294	0.03615879	0.25421073
C	0.35579668	0.81517389	1.00355377
C	2.61705638	−0.17836268	0.30117604
C	3.13073630	−0.99011925	−0.73201836
C	4.48840786	−1.29416973	−0.78817418
C	5.37224561	−0.79252880	0.17797451
C	4.86013049	0.00909077	1.19800836
C	3.49977127	0.32192010	1.27490611
C	−2.18651602	1.16478353	0.91319843
C	−3.30003902	0.60222592	0.25448612
C	−4.58693761	1.06842596	0.51026291
C	−4.80083031	2.10171143	1.43374930
C	−3.69714822	2.65544448	2.08227874
C	−2.39687130	2.20495922	1.83591392
F	−5.41816685	−0.22218935	−1.33555214
H	2.45843694	−1.38667790	−1.48803926

S	0.79998190	1.83285680	2.25641470
H	−1.03779282	−0.07848470	−0.18665195
H	3.11776807	0.94486381	2.07143909
H	0.79223324	−0.48412247	−0.50596904
C	5.02172399	−2.12368163	−1.93015744
H	6.43011935	−1.03138878	0.13260995
F	−6.74685631	1.31936721	−0.48827194
H	−3.15055584	−0.19905152	−0.46413900
C	−5.76626269	0.41785202	−0.16987515
H	−5.80482673	2.46401097	1.63107927
H	−1.55137766	2.64392904	2.34669382
F	5.54116963	−1.33795171	−2.93521384
F	4.05325114	−2.90500020	−2.51430481
F	6.02862173	−2.96493084	−1.53756771
F	−6.35824580	−0.53407016	0.63058334
H	−3.84423212	3.46154157	2.79709358
H	5.53040996	0.40169897	1.95890960
H	−0.17954655	−2.67711109	−3.25910577
H	−2.00359903	−2.32474359	−2.89863577
C	−0.93818476	−2.14949652	−2.64622722
O	−0.61510564	−1.40928258	−1.73495602

Formaldehyde–1,3-bis[3-(trifluoromethyl)phenyl]selenourea

E: −5273.48
H: −5102.81
G: −5148.41
N_{imag} = 0

N	0.05068670	1.12932955	0.36387432
N	−0.05068670	−1.12932955	0.36387432
C	−0.00000000	−0.00000000	1.15468111
C	−0.21294794	−2.49562229	0.68036322
C	0.31566766	−3.41173652	−0.24545370
C	0.15539263	−4.78454210	−0.05052489
C	−0.51989320	−5.26777972	1.07748801
C	−1.04862306	−4.35187186	1.98963514
C	−0.91079299	−2.97496174	1.80158445
C	0.21294794	2.49562229	0.68036322
C	−0.31566766	3.41173652	−0.24545370
C	−0.15539263	4.78454210	−0.05052489
C	0.51989320	5.26777972	1.07748801
C	1.04862306	4.35187186	1.98963514
C	0.91079299	2.97496174	1.80158445
F	−0.84694408	5.22572983	−2.30333253
H	0.85219590	−3.04741731	−1.11757252
Se	0.00000000	0.00000000	2.99647198
H	−0.14501675	0.97710345	−0.62490900
H	−1.33025293	−2.27507505	2.51169097
H	0.14501675	−0.97710345	−0.62490900
C	0.77347904	−5.74802677	−1.03328423
H	−0.63845700	−6.33583388	1.22972142
F	−0.07529258	6.92210222	−1.12525262
H	−0.85219590	3.04741731	−1.11757252
C	−0.77347904	5.74802677	−1.03328423
H	0.63845700	6.33583388	1.22972142
H	1.33025293	2.27507505	2.51169097
F	2.06130900	−6.08605015	−0.68158013
F	0.84694408	−5.22572983	−2.30333253
F	0.07529258	−6.92210222	−1.12525262
F	−2.06130900	6.08605015	−0.68158013
H	1.58962478	4.71326929	2.86072641
H	−1.58962478	−4.71326929	2.86072641
H	0.26696135	−0.90774590	−4.26547080
H	−0.26696135	0.90774590	−4.26547080

C	0.00000000	−0.00000000	−3.68707115
O	0.00000000	−0.00000000	−2.46948305

Formaldehyde–1,3-bis[3,5-bis(trifluoromethyl)phenyl]urea

E: −6164.47
H: −5982.69
G: −6038.97
N_{imag} = 0

H	−2.84625191	−0.05379943	3.97625614
H	−4.89489854	−0.05499483	3.97625304
N	−5.02343068	−0.06273296	2.96742562
C	−3.87057256	−0.05442479	2.17785454
H	−7.05267928	−0.04798157	4.59002750
N	−2.71771728	−0.04607840	2.96742894
H	−1.73995370	0.00573026	0.41425462
O	−3.87056930	−0.05443441	0.95127873
C	−1.38150003	−0.03437292	2.53976736
C	−0.39397619	−0.04501952	3.54435410
C	0.95625680	−0.02536141	3.20602744
C	1.36018423	0.00015245	1.86574433
C	0.37536466	0.01152327	0.87700857
C	−0.98777107	−0.00692195	1.19131152
H	−0.68846437	−0.06083123	4.59003094
C	2.00164408	−0.08775287	4.29617793
H	2.41128378	0.02073431	1.60348295
C	0.76928335	0.00599216	−0.58605054
C	−6.35964774	−0.07443681	2.53976242
C	−6.75338011	−0.10190237	1.19130841
C	−8.11651799	−0.12031892	0.87700832
C	−9.10133444	−0.10893949	1.86574543
C	−8.69740310	−0.08346515	3.20602888
C	−7.34717021	−0.06377906	3.54435130
H	−6.00119968	−0.11452065	0.41424850
C	−8.51042896	−0.11479193	−0.58605288
H	−10.15243438	−0.12952223	1.60348662
C	−9.74279029	−0.02113231	4.29618262
F	−8.32282152	1.12456933	−1.14965129
F	−9.82535447	−0.44091350	−0.77493812
F	−7.76566750	−0.99720859	−1.32120397
F	2.08414742	0.33236140	−0.77494414
F	0.58192908	−1.23344212	−1.14957589
F	0.02435351	0.88821441	−1.32125995
F	2.42588820	−1.37778117	4.51596089
F	1.53076333	0.37672316	5.49912180
F	3.11469952	0.64432188	3.98992935
F	−10.16708208	1.26887694	4.51598153
F	−9.27189124	−0.48560393	5.49912099
F	−10.85582058	−0.75324299	3.98992614
C	−3.87057802	−0.05438139	7.00502259
O	−3.87057756	−0.05438784	5.78709157
H	−4.81640363	−0.05266208	7.58344124
H	−2.92475280	−0.05609983	7.58344187

***C_{2v}* symmetry enforced**
E: −6164.31
H: −5983.15
G: −6037.12
N_{imag} = 4 (−5.7; −6.0; −6.2; −7.3 cm^{-1})

H	1.02250541	0.00000000	1.38235625
H	−1.02250541	0.00000000	1.38235625
N	−1.15253537	0.00000000	0.37363306
C	−0.00000000	0.00000000	−0.41666650

H	−3.18211674	0.00000000	1.99725311
N	1.15253537	0.00000000	0.37363306
H	2.13140298	0.00000000	−2.17968708
O	−0.00000000	0.00000000	−1.64328007
C	2.48998555	0.00000000	−0.05042175
C	3.47551039	0.00000000	0.95014550
C	4.83008190	0.00000000	0.61014191
C	5.23131753	0.00000000	−0.72532074
C	4.24212985	0.00000000	−1.71742078
C	2.88377876	0.00000000	−1.40405837
H	3.18211674	0.00000000	1.99725311
C	5.84560695	0.00000000	1.72960261
H	6.28284966	0.00000000	−0.98830178
C	4.68906191	0.00000000	−3.16473588
C	−2.48998555	0.00000000	−0.05042175
C	−2.88377876	0.00000000	−1.40405837
C	−4.24212985	0.00000000	−1.71742078
C	−5.23131753	0.00000000	−0.72532074
C	−4.83008190	0.00000000	0.61014191
C	−3.47551039	0.00000000	0.95014550
H	−2.13140298	0.00000000	−2.17968708
C	−4.68906191	0.00000000	−3.16473588
H	−6.28284966	0.00000000	−0.98830178
C	−5.84560695	0.00000000	1.72960261
F	−5.46176589	1.10034866	−3.45023031
F	−5.46176589	−1.10034866	−3.45023031
F	−3.64910062	0.00000000	−4.04483698
F	5.46176589	1.10034866	−3.45023031
F	5.46176589	−1.10034866	−3.45023031
F	3.64910062	0.00000000	−4.04483698
F	5.70135442	−1.09979642	2.54467826
F	5.70135442	1.09979642	2.54467826
F	7.13203689	0.00000000	1.28058648
F	−5.70135442	1.09979642	2.54467826
F	−5.70135442	−1.09979642	2.54467826
F	−7.13203689	0.00000000	1.28058648
C	−0.00000000	0.00000000	4.41131358
O	−0.00000000	0.00000000	3.19337973
H	−0.94577903	0.00000000	4.98979515
H	0.94577903	0.00000000	4.98979515

Formaldehyde–1,3-bis[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −6081.27
H: −5901.44
G: −5956.41
N_{imag} = 0

H	−0.16306477	−0.96533739	1.12358460
H	0.16306477	0.96533739	1.12358460
N	0.00299116	1.13279501	0.13155202
C	0.00000000	−0.00000000	−0.67231653
H	0.77834192	2.99363012	1.74610743
N	−0.00299116	−1.13279501	0.13155202
H	0.93947786	−2.35590241	−2.15113500
S	0.00000000	−0.00000000	−2.34127943
C	0.06257729	−2.50157033	−0.18418685
C	−0.38132521	−3.38800348	0.81455216
C	−0.31105357	−4.76633892	0.62065997
C	0.18817512	−5.29506591	−0.57363964
C	0.63461730	−4.40899815	−1.55749232
C	0.58290351	−3.02374531	−1.38012351
H	−0.77834192	−2.99363012	1.74610743
C	−0.83782155	−5.69130886	1.69404052
H	0.24215842	−6.36681571	−0.72554021

C	1.15207985	−4.95856422	−2.87110835
C	−0.06257729	2.50157033	−0.18418685
C	−0.58290351	3.02374531	−1.38012351
C	−0.63461730	4.40899815	−1.55749232
C	−0.18817512	5.29506591	−0.57363964
C	0.31105357	4.76633892	0.62065997
C	0.38132521	3.38800348	0.81455216
H	−0.93947786	2.35590241	−2.15113500
C	−1.15207985	4.95856422	−2.87110835
H	−0.24215842	6.36681571	−0.72554021
C	0.83782155	5.69130886	1.69404052
F	−0.13989444	5.08857489	−3.79136343
F	−1.71280487	6.19976393	−2.72532583
F	−2.09910940	4.15082991	−3.43590863
F	1.71280487	−6.19976393	−2.72532583
F	0.13989444	−5.08857489	−3.79136343
F	2.09910940	−4.15082991	−3.43590863
F	−2.18298622	−5.93091442	1.54142218
F	−0.67843444	−5.16515689	2.95367203
F	−0.21653902	−6.90762137	1.68465936
F	2.18298622	5.93091442	1.54142218
F	0.67843444	5.16515689	2.95367203
F	0.21653902	6.90762137	1.68465936
C	−0.00000000	−0.00000000	4.17466944
O	−0.00000000	−0.00000000	2.95655845
H	0.26148519	0.90916412	4.75262215
H	−0.26148519	−0.90916412	4.75262215

C_{2v} symmetry enforced
E: −6081.00
H: −5901.09
G: −5956.26
N_{imag} = 6 (−8.8; −9.9; −10.9 −13.4; −13.5; −14.1 cm^{-1})

H	0.94885540	0.00000000	1.03489333
H	−0.94885540	−0.00000000	1.03489333
N	−1.13152530	0.00000000	0.03289127
C	0.00000000	−0.00000000	−0.77388354
H	−2.91402575	−0.00000000	1.88154573
N	1.13152530	−0.00000000	0.03289127
H	2.45970883	−0.00000000	−2.40053103
S	0.00000000	0.00000000	−2.44417857
C	2.50974212	−0.00000000	−0.24251165
C	3.35077864	−0.00000000	0.88565130
C	4.73814415	−0.00000000	0.74120099
C	5.32332347	−0.00000000	−0.52546146
C	4.48181753	−0.00000000	−1.64404044
C	3.09210197	−0.00000000	−1.52475634
H	2.91402575	0.00000000	1.88154573
C	5.58453298	0.00000000	1.99358750
H	6.40139658	−0.00000000	−0.63873523
C	5.12358586	0.00000000	−3.01674841
C	−2.50974212	0.00000000	−0.24251165
C	−3.09210197	0.00000000	−1.52475634
C	−4.48181753	0.00000000	−1.64404044
C	−5.32332347	0.00000000	−0.52546146
C	−4.73814415	0.00000000	0.74120099
C	−3.35077864	0.00000000	0.88565130
H	−2.45970883	0.00000000	−2.40053103
C	−5.12358586	−0.00000000	−3.01674841
H	−6.40139658	0.00000000	−0.63873523
C	−5.58453298	−0.00000000	1.99358750
F	−5.92789139	1.10034949	−3.19294218
F	−5.92789139	−1.10034949	−3.19294218
F	−4.21392470	−0.00000000	−4.03060124

F	5.92789139	1.10034949	−3.19294218
F	5.92789139	−1.10034949	−3.19294218
F	4.21392470	0.00000000	−4.03060124
F	5.32551027	−1.09969657	2.78019390
F	5.32551027	1.09969657	2.78019390
F	6.92112199	0.00000000	1.73156037
F	−5.32551027	1.09969657	2.78019390
F	−5.32551027	−1.09969657	2.78019390
F	−6.92112199	−0.00000000	1.73156037
C	0.00000000	0.00000000	4.09391448
O	0.00000000	−0.00000000	2.87558889
H	−0.94586984	0.00000000	4.67183125
H	0.94586984	−0.00000000	4.67183125

Formaldehyde–1,3-bis[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −6059.59
H: −5880.29
G: −5935.88
$N_{imag} = 0$

H	−0.21862778	−0.99217372	1.27411188
H	0.21862778	0.99217372	1.27411188
N	0.00946360	1.13398771	0.28611229
C	0.00000000	−0.00000000	−0.49979239
H	1.29862218	3.06655476	1.47417451
N	−0.00946360	−1.13398771	0.28611229
H	1.47432550	−2.24039428	−1.71292951
Se	0.00000000	−0.00000000	−2.33772972
C	0.07042182	−2.49139515	−0.09203797
C	−0.66058200	−3.41527739	0.66655583
C	−0.58818288	−4.78035451	0.37254014
C	0.20264502	−5.24004238	−0.68161901
C	0.93912466	−4.31000852	−1.42498023
C	0.88791965	−2.94481049	−1.13970038
H	−1.29862218	−3.06655476	1.47417451
C	−1.34485151	−5.75597942	1.24356920
H	0.25206138	−6.29745761	−0.91465616
C	1.78059849	−4.79495867	−2.58626176
C	−0.07042182	2.49139515	−0.09203797
C	−0.88791965	2.94481049	−1.13970038
C	−0.93912466	4.31000852	−1.42498023
C	−0.20264502	5.24004238	−0.68161901
C	0.58818288	4.78035451	0.37254014
C	0.66058200	3.41527739	0.66655583
H	−1.47432550	2.24039428	−1.71292951
C	−1.78059849	4.79495867	−2.58626176
H	−0.25206138	6.29745761	−0.91465616
C	1.34485151	5.75597942	1.24356920
F	−1.03480511	4.90609725	−3.73433441
F	−2.31918842	6.03279844	−2.34738984
F	−2.81792915	3.95023759	−2.86665148
F	2.31918842	−6.03279844	−2.34738984
F	1.03480511	−4.90609725	−3.73433441
F	2.81792915	−3.95023759	−2.86665148
F	−2.57498876	−5.27189602	1.61173398
F	−0.66569375	−6.01364621	2.41544864
F	−1.54830407	−6.95884817	0.63303229
F	2.57498876	5.27189602	1.61173398
F	0.66569375	6.01364621	2.41544864
F	1.54830407	6.95884817	0.63303229
C	0.00000000	−0.00000000	4.31681001
O	−0.00000000	−0.00000000	3.09873131
H	0.33417087	0.88491974	4.89513701
H	−0.33417087	−0.88491974	4.89513701

***C*$_{2v}$ symmetry enforced**
E: −6058.87
H: −5879.91
G: −5933.79
N_{imag} = 6 (−8.1; −9.3; −10.0; −11.9; −14.9; −15.1 cm^{-1})

H	0.94017144	0.00000000	0.98536820
H	−0.94017144	−0.00000000	0.98536820
N	−1.12800126	−0.00000000	−0.01663463
C	0.00000000	0.00000000	−0.81756555
H	−2.87211020	−0.00000000	1.86314494
N	1.12800126	0.00000000	−0.01663463
H	2.50431446	−0.00000000	−2.42670295
Se	0.00000000	0.00000000	−2.65652610
C	2.51204769	−0.00000000	−0.26896379
C	3.32939730	0.00000000	0.87648209
C	4.71933356	0.00000000	0.76093451
C	5.33038637	−0.00000000	−0.49366808
C	4.51206833	−0.00000000	−1.62913286
C	3.12022807	−0.00000000	−1.53821977
H	2.87211020	0.00000000	1.86314494
C	5.53937670	0.00000000	2.03064432
H	6.41061704	−0.00000000	−0.58469889
C	5.18073150	−0.00000000	−2.98902736
C	−2.51204769	0.00000000	−0.26896379
C	−3.12022807	0.00000000	−1.53821977
C	−4.51206833	0.00000000	−1.62913286
C	−5.33038637	0.00000000	−0.49366808
C	−4.71933356	−0.00000000	0.76093451
C	−3.32939730	−0.00000000	0.87648209
H	−2.50431446	0.00000000	−2.42670295
C	−5.18073150	0.00000000	−2.98902736
H	−6.41061704	0.00000000	−0.58469889
C	−5.53937670	−0.00000000	2.03064432
F	−5.98839991	1.10035337	−3.14918275
F	−5.98839991	−1.10035337	−3.14918275
F	−4.29095385	0.00000000	−4.02002597
F	5.98839991	1.10035337	−3.14918275
F	5.98839991	−1.10035337	−3.14918275
F	4.29095385	−0.00000000	−4.02002597
F	5.26382827	−1.09967487	2.81176008
F	5.26382827	1.09967487	2.81176008
F	6.88101296	0.00000000	1.79658223
F	−5.26382827	1.09967487	2.81176008
F	−5.26382827	−1.09967487	2.81176008
F	−6.88101296	−0.00000000	1.79658223
C	0.00000000	0.00000000	4.04865235
O	0.00000000	0.00000000	2.83014374
H	−0.94587956	0.00000000	4.62641112
H	0.94587956	−0.00000000	4.62641112

Formaldehyde–1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]urea

E: −5376.46
H: −5202.98
G: −5251.39
N_{imag} = 0

N	−0.89608056	−1.06096431	−0.07995655
N	−0.82598198	1.24078745	−0.00072550
C	−0.09439564	0.06876543	0.15004694
C	−0.38579265	2.57548452	0.14395318
C	−1.34395274	3.58589320	−0.07092339
C	−0.99467677	4.92992563	0.05121398

C	0.31487625	5.29089737	0.38947577
C	1.26389697	4.28641303	0.60216558
C	0.93101177	2.93364086	0.48401443
C	−0.52375364	−2.40670750	−0.02020827
C	−1.52461546	−3.35801580	−0.30601084
C	−1.24234903	−4.72013574	−0.25917848
C	0.04062196	−5.17707877	0.06573233
C	1.02720469	−4.22998666	0.34726731
C	0.76813294	−2.85612516	0.30855731
C	2.43721442	−4.68117704	0.66716217
H	−2.36433475	3.31026394	−0.33479799
O	1.09629656	0.01419509	0.44460257
H	−1.87258581	−0.89363702	−0.31593755
H	1.66933062	2.16071803	0.64951095
H	−1.80637828	1.14416078	−0.24612587
H	−1.74834887	5.69564132	−0.11871722
H	0.58926637	6.33845119	0.48507251
H	2.28537047	4.55253646	0.86549409
H	−2.52676769	−3.02381998	−0.55831124
C	−2.31801051	−5.71844977	−0.61721846
H	0.25882051	−6.23752418	0.10710091
H	1.54094990	−2.13329865	0.53290258
H	−5.65712158	0.13424392	−1.03173214
H	−4.95559023	−1.61677169	−0.89955645
C	−4.77694011	−0.52166949	−0.87433897
O	−3.66779126	−0.05838052	−0.68275845
F	3.27613645	−4.50547009	−0.40820371
F	2.49973431	−6.00671044	1.00299132
F	2.98102450	−3.97639908	1.70710787
F	−2.23643812	−6.10277706	−1.93597416
F	−3.58366783	−5.21121342	−0.44063398
F	−2.23738788	−6.86131905	0.12873879

Formaldehyde–1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: −5293.77
H: −5121.60
G: −5170.72
N_{imag} = 0

N	−0.67144979	−0.99490727	−0.00473801
N	−0.54099844	1.26529960	−0.00882838
C	0.17560588	0.09945260	−0.18328667
C	−0.22228520	2.63475286	−0.16845300
C	−1.31217396	3.52559061	−0.06969786
C	−1.12048928	4.89941586	−0.19308455
C	0.16213566	5.41380385	−0.41977010
C	1.24099476	4.53112946	−0.51540855
C	1.06616261	3.14915690	−0.39030487
C	−0.39744977	−2.36879030	0.02901370
C	−1.45489180	−3.22941793	−0.31198844
C	−1.30323885	−4.61429075	−0.22474111
C	−0.08868666	−5.17442863	0.17550123
C	0.96303908	−4.31234070	0.50958415
C	0.82580235	−2.92482899	0.44792565
C	2.29490251	−4.90671745	0.91654853
H	−2.31307849	3.13039116	0.10105004
S	1.79403818	−0.02493122	−0.58456388
H	−1.67124462	−0.78637540	0.00614862
H	1.90759749	2.47452638	−0.46428472
H	−1.51939541	1.13251251	0.23648211
H	−1.97485449	5.56783300	−0.11479865
H	0.31516631	6.48553835	−0.51886253
H	2.24357036	4.91629565	−0.68813415
H	−2.39721429	−2.80977496	−0.65294184

C	−2.46633984	−5.49318833	−0.61792020
H	0.03248537	−6.24934498	0.23995459
H	1.64592567	−2.27698072	0.72303778
H	−5.42372145	−0.44753601	1.01801323
H	−4.39013616	−1.98472216	0.63657990
C	−4.45737773	−0.87819307	0.68618182
O	−3.51560712	−0.16402800	0.39132770
F	3.06765055	−5.20365937	−0.18081394
F	2.14266490	−6.07742058	1.61495730
F	3.02882518	−4.06248915	1.70100586
F	−2.61233573	−5.57213100	−1.98230028
F	−3.66241981	−5.00129600	−0.13462575
F	−2.34537460	−6.77037789	−0.15589374

Formaldehyde–1-phenyl-3-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −5272.06
H: −5100.99
G: −5148.90
N_{imag} = 0

N	−0.76886128	−0.94643751	−0.14061027
N	−0.69168936	1.30991148	0.00176507
C	0.05626828	0.15695166	−0.01927190
C	−0.29761843	2.67429841	0.00095473
C	−1.11796913	3.57513038	0.70123448
C	−0.82378348	4.93959989	0.70420494
C	0.29483578	5.41781056	0.01329610
C	1.10359725	4.51890224	−0.69061457
C	0.81386905	3.15250659	−0.70872878
C	−0.48080889	−2.31880542	−0.06011086
C	−1.29944069	−3.18189967	−0.80287455
C	−1.13455977	−4.56738224	−0.71558315
C	−0.13479859	−5.11511619	0.08829123
C	0.68080294	−4.24632138	0.82596404
C	0.51770275	−2.86192132	0.76893528
C	1.78137627	−4.83350025	1.68344453
H	−1.98038042	3.20050819	1.25058684
Se	1.89156923	0.07534210	0.08234873
H	−1.73591464	−0.75587452	−0.41526270
H	1.44135643	2.46217011	−1.25732615
H	−1.69042228	1.18159577	0.15197212
H	−1.46459445	5.62516925	1.25371771
H	0.53116271	6.47901780	0.02071350
H	1.96908553	4.88177911	−1.24034045
H	−2.05883565	−2.76616514	−1.45934025
C	−2.04597622	−5.44808230	−1.53502324
H	−0.00172857	−6.18874042	0.15281683
H	1.14385112	−2.20653056	1.35808872
H	−5.61598907	−0.95447901	−0.24557401
H	−4.34763824	−2.31422071	−0.59065323
C	−4.55818121	−1.23818019	−0.42042939
O	−3.67265150	−0.40147323	−0.42311922
F	2.18706706	−3.98421306	2.67282939
F	−1.78532540	−5.34907640	−2.88028329
F	−3.37131089	−5.08698030	−1.37786768
F	−1.95189239	−6.76664916	−1.20448603
F	2.89354365	−5.13590283	0.93476646
F	1.38999200	−6.00191421	2.28830249

Formaldehyde–1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]urea

E: −5887.63
H: −5671.38
G: −5719.66
N_{imag} = 0

H	2.92222317	3.83977740	3.42019201
H	2.55835802	4.43777676	1.80291041
H	4.68840259	2.34001763	2.51196857
H	4.99945632	3.99753681	1.99342275
N	0.92408765	0.83850798	0.46190374
N	-1.16655339	-0.13157741	0.25292494
C	-0.42365677	1.06187699	0.27866575
C	-2.53683564	-0.28972768	0.04686322
C	-3.04298149	-1.60549290	0.07222635
C	-4.39788373	-1.85056797	-0.13615533
C	-5.29101765	-0.79844890	-0.36738419
C	-4.78520311	0.50426262	-0.38396781
C	-3.42884497	0.77561010	-0.18357420
C	-5.71403237	1.66165997	-0.68443296
F	-3.95483988	-4.19567953	-0.37560837
F	-5.65223822	2.02411934	-2.01094781
F	-5.40494136	2.77890355	0.04133737
F	-7.02479221	1.36103507	-0.42234201
F	-5.98099700	-3.48619595	-0.87731288
F	-5.33595247	-3.57938686	1.22369838
H	-2.36787943	-2.43608432	0.25499142
O	-0.91667524	2.18110300	0.13266430
H	1.24084568	-0.09519432	0.70335604
H	-3.04826669	1.78825332	-0.20023785
H	-0.64170995	-0.99617784	0.37766491
C	-4.91609153	-3.26611125	-0.04942978
H	-6.34528075	-0.98910248	-0.52862055
C	1.86180903	1.94738569	0.67698063
C	4.28058430	2.68644275	0.41062894
C	3.26630516	1.54614407	0.19308344
C	1.88811924	2.40730681	2.15112383
C	2.89729032	3.55236574	2.36139020
C	4.30539941	3.15501134	1.87854864
H	1.49283216	2.77799057	0.06380840
H	4.00833565	3.53497012	-0.23469907
H	5.27987237	2.35968203	0.09576479
H	3.59648433	0.65563604	0.75255543
H	3.22176960	1.26347416	-0.86619573
H	2.16696392	1.54838105	2.78135404
H	0.87933376	2.71735113	2.44667477
C	0.52140284	-3.67174702	0.42798003
H	1.35024815	-4.39851516	0.55240838
H	-0.46070657	-4.08282607	0.11208256
O	0.68550212	-2.48286740	0.62876908

Formaldehyde–1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]thiourea

E: -5808.04
H: -5592.41
G: -5642.94
N_{imag} = 0

H	3.24190478	3.46185494	3.66895377
H	2.77147822	4.31472049	2.20015066
H	4.83703712	2.04702330	2.38615602
H	5.19302706	3.74980564	2.09150451
N	0.83395765	1.04281387	0.50227022
N	-1.21774115	0.08110704	0.27530329
C	-0.51108425	1.26996737	0.42515393
C	-2.57941689	-0.16941682	0.06833265
C	-3.03374067	-1.46173131	0.38877651
C	-4.35695934	-1.83291025	0.14959148
C	-5.26817022	-0.92106117	-0.38856972
C	-4.81256610	0.36511657	-0.69994759

C	−3.48797512	0.75173436	−0.48625911
C	−5.79408961	1.37764742	−1.25136895
F	−3.83788144	−4.16864265	0.21788938
F	−5.19012561	2.32440814	−2.02953014
F	−6.44369119	2.04807562	−0.24167960
F	−6.76792244	0.78741973	−2.01652017
F	−5.94819009	−3.60756902	−0.09205395
F	−5.01580375	−3.34358986	1.88355129
H	−2.34549940	−2.17459574	0.83375182
S	−1.19542668	2.80202904	0.52545892
H	1.16194314	0.08046702	0.48037606
H	−3.15120297	1.74736689	−0.74046858
H	−0.66678826	−0.77047435	0.39581968
C	−4.79660175	−3.22565252	0.53125790
H	−6.29698485	−1.20667144	−0.57301998
C	1.84702398	2.06564228	0.78824426
C	4.26863192	2.72681050	0.40704923
C	3.17684037	1.67721566	0.11855290
C	2.02389189	2.28533196	2.30563839
C	3.10932198	3.34152941	2.58635955
C	4.44603128	2.96428614	1.91942173
H	1.47364177	2.99634544	0.34547255
H	3.98967412	3.67422617	−0.07741041
H	5.21665266	2.40887611	−0.04511034
H	3.50374462	0.69807266	0.50525576
H	3.02492955	1.56491070	−0.96250021
H	2.30820444	1.32824397	2.76949245
H	1.06269123	2.58857753	2.73464197
C	0.28958456	−3.45575235	−0.01543448
H	1.06899208	−4.22923133	−0.17190555
H	−0.76353499	−3.76260124	−0.18450259
O	0.58208801	−2.32386914	0.32585928

Formaldehyde–1-cyclohexyl-3-[3,5-bis(trifluoromethyl)phenyl]selenourea

E: −5787.11
H: −5571.85
G: −5623.11
N_{imag} = 0

H	3.29175741	3.29963813	3.75069754
H	2.75639569	4.24638345	2.36377331
H	4.87897877	2.02415875	2.32035983
H	5.18618253	3.75242347	2.14289403
N	0.84286432	1.06169594	0.48754251
N	−1.18830636	0.06657024	0.25208799
C	−0.50158619	1.25132124	0.44033224
C	−2.55484894	−0.18671871	0.05852298
C	−3.03039805	−1.44059784	0.47227154
C	−4.36073461	−1.80604920	0.24932476
C	−5.24876680	−0.92117861	−0.36313498
C	−4.76782629	0.32977406	−0.77178148
C	−3.43781357	0.70505342	−0.57824837
C	−5.73002318	1.30545379	−1.41451686
F	−3.94806138	−4.16028322	0.29609671
F	−5.09721164	2.23921226	−2.18417040
F	−6.45549835	1.99171990	−0.46966606
F	−6.64314442	0.66983152	−2.21907756
F	−6.05336043	−3.50333227	0.25712972
F	−4.85351521	−3.25700095	2.08629628
H	−2.35861511	−2.12601334	0.98165117
Se	−1.29085902	2.91213143	0.65445529
H	1.19412224	0.10963012	0.40449957
H	−3.07837967	1.66887897	−0.91205388
H	−0.63251162	−0.78619883	0.35377005

C	−4.81444083	−3.16769960	0.71509522
H	−6.28205177	−1.20061250	−0.53209293
C	1.84330603	2.08600432	0.81626987
C	4.23430356	2.83332035	0.41458349
C	3.15901924	1.78001730	0.08033845
C	2.05971025	2.19705379	2.33971516
C	3.12882509	3.25649709	2.66644154
C	4.45259232	2.96307031	1.93465991
H	1.43249649	3.03573160	0.45415377
H	3.91791866	3.80619908	0.01037815
H	5.17498009	2.57406263	−0.08745392
H	3.52060608	0.78356712	0.38305499
H	2.97597098	1.74461508	−1.00110879
H	2.37909171	1.21612154	2.72431457
H	1.10452358	2.44533836	2.81526809
C	0.17604882	−3.47408060	−0.13770162
H	0.90477682	−4.28382713	−0.34607267
H	−0.89831615	−3.71798923	−0.27067968
O	0.54464870	−2.36959198	0.22038185

Formaldehyde–5,6-dihydroindolo[2,3-*b*]indole (X = C; R = 3-CF_3-phenyl)

E: −5240.42
H: −5079.49
G: −5127.24
N_{imag} = 0

H	−0.02980627	−1.50621711	−2.94640037
H	0.02980627	1.50621711	−2.94640037
N	0.02286265	1.27013866	−1.96204894
C	0.00000000	0.00000000	−1.44850495
H	0.07231487	4.11426382	−1.79068591
N	−0.02286265	−1.27013866	−1.96204894
F	1.43503106	6.14350358	0.67478496
C	−0.00000000	−0.00000000	−0.04675833
C	−0.04127194	−2.15659986	−0.86542091
C	−0.06502137	−3.54474286	−0.86622881
C	−0.07166312	−4.19535136	0.37673955
C	−0.06128527	−3.46451766	1.58278624
C	−0.03760542	−2.07080693	1.57712805
C	−0.02693506	−1.38354291	0.35262311
H	−0.07231487	−4.11426382	−1.79068591
C	−0.15019841	−5.69547001	0.43172725
H	−0.06602588	−4.00022709	2.52731319
F	0.24472958	−6.29196017	−0.74124187
C	0.04127194	2.15659986	−0.86542091
C	0.02693506	1.38354291	0.35262311
C	0.03760542	2.07080693	1.57712805
C	0.06128527	3.46451766	1.58278624
C	0.07166312	4.19535136	0.37673955
C	0.06502137	3.54474286	−0.86622881
F	−0.62831134	6.22760458	1.43029944
F	−1.43503106	−6.14350358	0.67478496
H	0.06602588	4.00022709	2.52731319
C	0.15019841	5.69547001	0.43172725
F	0.62831134	−6.22760458	1.43029944
F	−0.24472958	6.29196017	−0.74124187
H	−0.02509117	−1.52295109	2.51559483
H	0.02509117	1.52295109	2.51559483
C	−0.00000000	−0.00000000	−5.92144713
O	−0.00000000	−0.00000000	−4.70464001
H	0.01984734	0.94473374	−6.50377182
H	−0.01984734	−0.94473374	−6.50377182

Formaldehyde–5,6-dihydroindolo[2,3-*b*]indole (X = Si; R = 3-CF_3-phenyl)

E: −5119.99
H: −4962.54
G: −5009.57
N_{imag} = 0

H	1.15176733	−2.11499704	0.50850642
H	−0.05384805	−2.70367874	−1.79626166
N	−0.14564053	−1.69146872	−1.86446196
C	0.39226819	−0.83503251	−0.96414815
H	−1.58995061	−2.76898891	−3.92409077
N	0.94855319	−1.15720714	0.22759036
F	−3.02992094	−2.85485506	−5.91698298
Si	−0.03357928	0.96756363	−1.20179091
C	0.82033641	−0.10998757	1.17811975
C	1.34171800	−0.19074534	2.46849750
C	1.09803595	0.86295185	3.35695899
C	0.37343734	1.99346806	2.94420239
C	−0.08904123	2.08498238	1.62967611
C	0.09223424	1.03673309	0.71346512
H	1.91880732	−1.05570275	2.78450768
C	1.56653078	0.75639422	4.78421696
H	0.18768524	2.80043587	3.64682310
F	2.64638577	−0.08049941	4.92534472
C	−1.17329388	−1.08342175	−2.63305192
C	−1.46986687	0.27401391	−2.27189648
C	−2.50289563	0.90639047	−2.98195694
C	−3.23854818	0.22967339	−3.95720395
C	−2.90639911	−1.09248938	−4.29649552
C	−1.85722274	−1.75279323	−3.64676082
F	−4.15773784	−1.00686079	−6.33578671
F	0.58209336	0.25452888	5.61304944
H	−4.05902187	0.72668945	−4.46633274
C	−3.72317929	−1.82641427	−5.32702751
F	1.92836582	1.96833416	5.31165388
F	−4.85622725	−2.39380331	−4.77734795
H	−0.61084528	2.98725552	1.31726548
H	−2.74782373	1.94390562	−2.76386750
C	0.80056224	−5.30826088	−0.04684043
O	0.77331895	−4.12424680	−0.32876559
H	0.38550326	−6.07758069	−0.72996102
H	1.24165989	−5.66848297	0.90522875

Formaldehyde–5,6-dihydroindolo[2,3-*b*]indole (X = Ge; R = 3-CF_3-phenyl)

E: −5090.21
H: −4933.23
G: −4981.34
N_{imag} = 0

H	1.16612582	−2.01294246	0.41722895
H	0.00496706	−2.57946700	−1.80341028
N	−0.07394301	−1.56753059	−1.91496719
C	0.44502596	−0.70365199	−1.02592474
H	−1.44703996	−2.73419737	−3.95842489
N	1.00497844	−1.04118540	0.14818589
F	−2.84453183	−2.85227200	−6.02651743
Ge	−0.01968623	1.23942584	−1.27849367
C	0.86016974	−0.03542238	1.15066554
C	1.41051070	−0.17950830	2.42333830
C	1.15722310	0.81403582	3.37836023
C	0.39618190	1.94349214	3.04532806
C	−0.09850091	2.09239838	1.74409482
C	0.08482727	1.09966666	0.77495249
H	2.02342866	−1.04130547	2.67490884
C	1.66179242	0.63057393	4.78571143

H	0.20197552	2.70403920	3.79593302
F	2.82794038	−0.09442511	4.83634979
C	−1.14332295	−1.01283692	−2.68057604
C	−1.53438163	0.30976750	−2.32179984
C	−2.59791026	0.87316182	−3.03568060
C	−3.29324127	0.14394596	−4.00778695
C	−2.87881532	−1.15452834	−4.33601838
C	−1.78432414	−1.73791857	−3.68384668
F	−4.25165572	−1.17674762	−6.29904134
F	0.75390338	−0.05228236	5.57192870
H	−4.14638041	0.58310994	−4.51646660
C	−3.64356748	−1.95878481	−5.35439542
F	1.90186137	1.81921095	5.42109462
F	−4.64531682	−2.70909312	−4.76920865
H	−0.65379675	2.99464276	1.49433714
H	−2.91067663	1.89370564	−2.82250693
C	0.51565632	−5.16377719	0.06859134
O	0.67606955	−4.01611001	−0.30500981
H	0.01241309	−5.91727258	−0.57127056
H	0.86626165	−5.50411374	1.06441199

Formaldehyde–1,3-bis[4-(trifluoromethyl)phenyl]urea

E: −5378.86
H: −5204.68
G: −5255.22
N_{imag} = 0

C	−0.17277054	−9.40809808	−1.80480641
C	−0.19559895	−10.75888850	−1.48070272
C	−0.21251419	−11.15786236	−0.13660601
C	−0.19974021	−10.18311102	0.86812575
C	−0.17711732	−8.82483828	0.55414633
C	−0.08798720	−3.43732779	−0.79512042
C	−0.07811611	−2.45122367	−1.80480471
C	−0.05526630	−1.10043375	−1.48070033
C	−0.03836599	−0.70146054	−0.13660324
C	−0.05117902	−1.67621181	0.86812815
C	−0.07382303	−3.03448404	0.55414811
H	−0.11587530	−4.98413223	−5.86101604
H	−0.16470137	−9.10465724	−2.85025514
O	−0.12548261	−5.92966119	0.80076348
H	−0.11325023	−4.90650717	−2.22409059
H	−0.17195659	−8.07634373	1.33452122
H	−0.13766984	−6.95281373	−2.22409116
C	−0.12545732	−5.92966428	−5.28098664
C	−0.18374949	−12.61988170	0.21361705
H	−0.03724192	−1.37524623	1.91155091
H	−0.08617067	−2.75466421	−2.85025363
O	−0.12545436	−5.92966062	−4.06416339
C	−0.06710192	0.76055937	0.21362001
H	−0.07901302	−3.78297864	1.33452272
H	−0.21368914	−10.48407705	1.91154820
H	−0.13504183	−6.87519986	−5.86101027
H	−0.04409510	−0.35501207	−2.27040875
H	−0.20673837	−11.50431029	−2.27041150
F	1.10430468	−13.11665947	0.26273760
F	−0.85231732	−13.39146852	−0.70607762
F	−0.74208539	−12.88077371	1.43751838
F	0.49122346	1.02143783	1.43752905
F	−1.35514533	1.25736700	0.26272349
F	0.60149624	1.53213113	−0.70606513
N	−0.10877369	−4.77616625	−1.21600003
N	−0.14216039	−7.08315506	−1.21600069

```
C      -0.12547441      -5.92966079      -0.42631370
C      -0.16293493      -8.42199389      -0.79512179
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