SUPPLEMENTARY MATERIAL

of the Article

Step-by-Step Replacement of Cyano Groups by Tricyanovinyls — The Influence on the Acidity

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1. Materials and Methods

1.1. Computational Gas-phase acidities

All electronic structure calculations in this study were performed with the quantum chemical program package Turbomole version 7.2 or Gaussian 16.

For all the compounds, frequency calculations were carried out to check for the presence of imaginary frequencies. These may indicate that found geometry corresponds to a transitional state rather than energy minimum. However, small negative frequencies may be an artifact of computational procedure. In some cases, imaginary frequencies were found, and geometries were adjusted and reoptimized to eliminate or reduce them. It was found that the effect of such corrections on the computed GA values was negligible.

Calculating the molecule as a cycle where the proton is attached between two CN groups did not lead to any stable species. During the geometry optimization, the ring is broken, or a structure with imaginary frequencies is obtained.

In the case of Gaussian B3LYP/6-311+G(d,p) results, the *H* and *G* values come straight from the output as "Sum of electronic and thermal Enthalpies" and "Sum of electronic and thermal Free Energies", respectively. In the case of G4(MP2) method, the H and G value comes from the output as "G4MP2(0 K)" and "G4MP2 Energy", respectively. W1RO and CBS-APNO final energies come from Gaussian outputs as "W1RO Enthalpy" and "W1RO Free Energy", and "CBS-APNO Enthalpy" and "CBS-APNO Free Energy", respectively. Gaussian calculations are performed at the temperature 298.2 K and at the pressure 1.0 atm.

In the case of Turbomole results, the *H* and *G* values need to be calculated for every species according to equations 2-3. Thermochemical properties (Enthalpy and Chemical potential) are available from the frequency calculations, where the following parameters are used: temperature 298.15 K, pressure 0.1 MPa, frequency scale 0.9914, sigma 1.0, symmetry C1.

$$H = \text{total energy} + \text{Enthalpy} \tag{S1}$$

$$G = \text{total energy} + \text{Chemical potential} \tag{S2}$$

Then, PA and GA are calculated as follows:

$$\text{PA} = H(\text{A}^-) + H(\text{H}^+) - H(\text{AH}) \tag{S3}$$

$$\text{GA} = G(\text{A}^-) + G(\text{H}^+) - G(\text{AH}) \tag{S4}$$

Where values for proton are: $H(\text{H}^+)$ = 1.481 kcal/mol; $G(\text{H}^+)$ = -6.275 kcal/mol.

1.2. Computational solution phase acidities

Acidities in the solution were estimated using either a correlation between pK_a values in two solvents or values computed with the COSMO-RS method and corrected using the available experimental data for similar compounds. The auxiliary acids that were chosen to correct computational pK_a values are all cyanocarbon acids measured in 1,2-dichloroethane (DCE). The obtained results are summarized in Table 4 in the main text and Table S8.

The COSMO-RS files were calculated for all the conformers of anions and all the conformers/isomers of the most stable tautomer of neutral form. For this, two sequenced COSMO calculations were performed. First, the structure was optimized in the ideal conductor using the BP86/def-TZVP basis set, and then the COSMO file with the FINE cavity parameter was calculated using the BP86/def2-TZVPD method. Using obtained cosmo files, a conformer set was created for anion and neutral species, and pK_a values in MeCN, DMSO, and H_2O were calculated using COSMOtherm software with parametrization BP_TZVPD_FINE_19. All unique conformers were considered. The conformational search was conducted only for anion **14** with COSMOconf software using BP-TZVP-GAS methods.

pK_a(DMSO) values in the current work are obtained from pK_a(MeCN) values by averaging two different values calculated from previously published pK_a(MeCN) vs pK_a(DMSO) correlation equations.[34,42 in the main text] Also, COSMO-RS pK_a(DMSO) values are available in Table S8. To correlate the assigned pK_a(DMSO) values with pKa(DMSO) COSMO-RS values, a very good correlation is obtained, however, the values themselves deviate from each other. The equation is as follows:

$$\text{p}K_a\text{(DMSO) ASSIGNED} = 1.299(0.015) \cdot \text{p}K_a\text{(DMSO) COSMO-RS} - 0.63(0.20) \quad (S5)$$

$$r^2=0.998;\ S=0.685;\ \text{n}=19$$

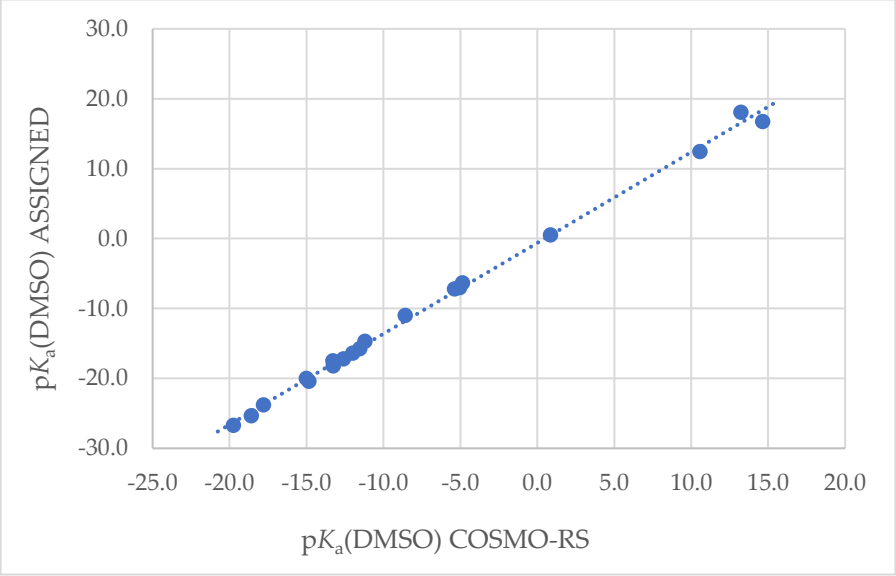


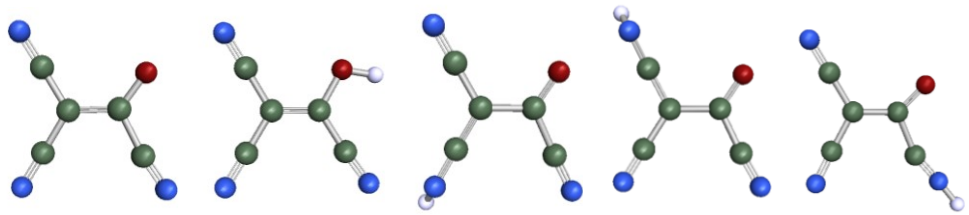
Figure S1. Correlation between pK_a(DMSO) values listed in Table S4 and computationally obtained COSMO-RS pK_a(DMSO) values according to Eq S5.

1.3. Structural Details

In the following sections, in comparison of energies of different tautomers and conformers, only data from calculations of BP86/def-TZVP basis set are used because other methods were not used to calculate the less stable forms. *Relative Gibbs free energy values* (ΔG) in the gas-phase are provided to compare the stability of different tautomers and conformers. The reader must note that it is not the GA value.

1.3.1. Central atom O

Divalent oxygen substituted with the CN group exhibits two tautomers: OH-acid (cyanic acid, **1H-T1**) and NH-acid (isocyanic acid **1H-T2**, Figure 7 in the main text). The replacement of the CN group with the TCNV group gives a structure with five possible tautomers (Figure S2). The most stable form is OH-acid, tautomer **T1**.

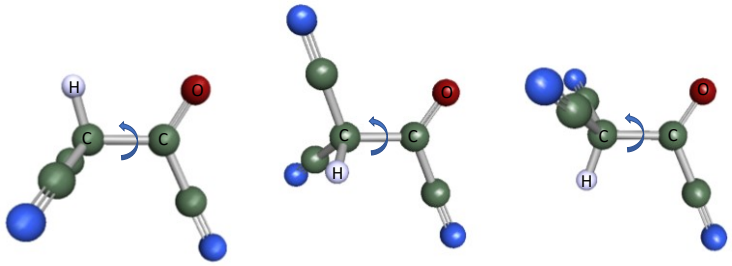


	2	**2H-T1**	**2H-T4**	**2H-T5**	**2H-T6**
Δ*G* [kcal/mol]		0	3.4	4.0	19.7

Figure S2. Geometries of **2** and its conjugate acids in different tautomeric forms with their Δ*G* values compared to the most stable **2H-T1**.

Anion **2** is planar. Tautomers **T1**, **T4**-**T5** are also planar, except the proton is bent out of the plane. In the case of **T6**, the C-N-H angle is almost straight (177°), but the C-C-N angle, where the proton is attached, is slightly bent (161°). The whole molecule, however, is fully planar.

Tautomers **T4** and **T5** have a similar energy, **T4** is 0.6 kcal/mol more stable. These tautomers are, respectively, 3.4 and 4.0 kcal/mol less stable than the most stable **T1**. The least stable form is **T6**, which is 19.7 kcal/mol less stable than **T1**. Tautomer **T3**, CH-acid, has different conformers since the possibility to rotate about the C-C bond. Two conformers are computationally archivable: *syn*(H) form and *eclipsed*(H) form (Figure S3). *Syn*(H) form is the most stable among CH-acids, 0.2 kcal/mol more stable than *eclipsed*(H) form. *Anti*(H) is not possible to obtain during structure optimization; however, when the torsion angle is frozen (179°) during the optimization, we obtain the structure which is 2.8 kcal/mol less stable than *syn*(H) form (imaginary frequencies are not zero). **T3** *syn*(H) form is 6.8 kcal/mol less stable than the most stable **2H-T1**.



	2H-T3 *syn*(H)	**2H-T3** *eclipsed*(H)	**2H-T3** *anti*(H)*
< ω(O-C-C-H) [°]	1.7	117.2	179*
Δ*G* [kcal/mol]	6.8	7.0	9.5

Figure S3. Three different conformers of compound **2H-T3** and their Δ*G* values compared to the most stable **2H-T1**. **Anti*(H) is not a stable conformer for this compound, having imaginary frequencies. Torsion angles (< ω) of O–C–C–H are presented.

1.3.2. Central atom N

The most stable tautomer of dicyanamine has a proton attached to the CN group nitrogen, tautomer **T2** (Figure 7 in the main text).

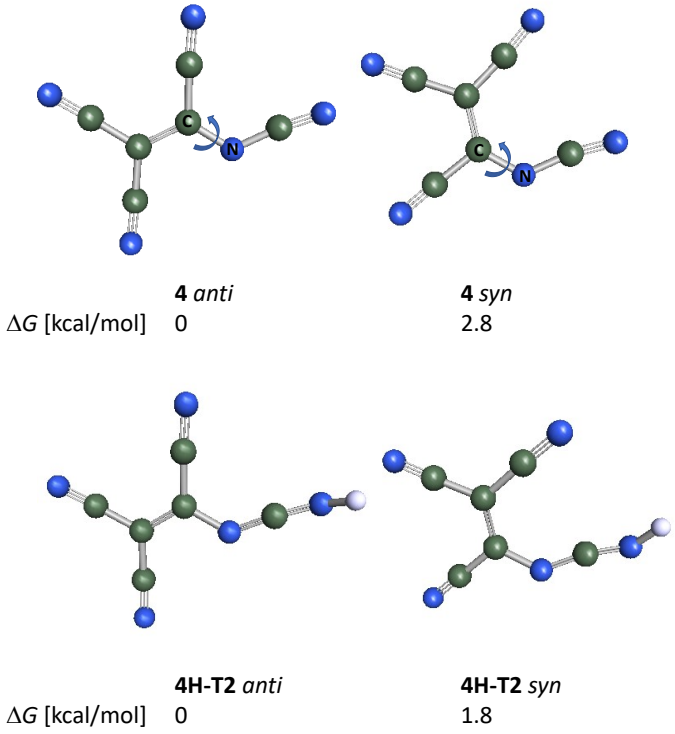


Figure S4. Geometry of **4** and its most stable tautomers **4H-T2**.

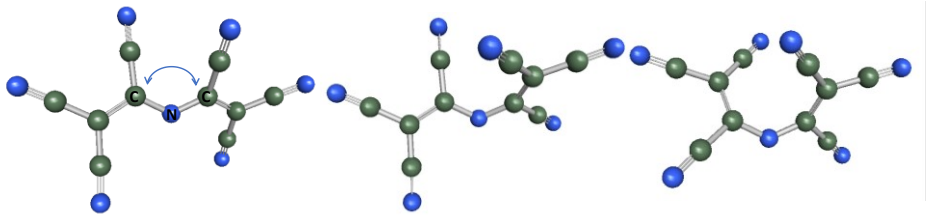
Its TCNV substituted analog, anion **4,** and its conjugate acids, **4H-T1**, **4H-T2,** and **4H-T6**, can be in *anti* and *syn* conformation. Acids **4H-T3**, **4H-T4**, and **4H-T5** exhibit *trans* and *cis* isomers (Figure S4). *Syn* and *cis* forms are less stable, most probably because of the repulsion between CN and TCNV groups. Anions in *anti* and *syn* conformation are fully planar. Acid forms, except tautomer **T3**, CH-acid, are also planar; only the proton is bent out of the plane. Acid **4H-T3**, differently from **2H-T3**, the *anti*(H) form is also stable; however, the lowest energy is obtained for *syn*(H) conformer (Table S1).

Table S1. Δ*G* values (kcal/mol) of the most stable conformers of different tautomers for compound **4H**, relative to the **4H-T2** *anti* conformer at BP86/def-TZVP level.

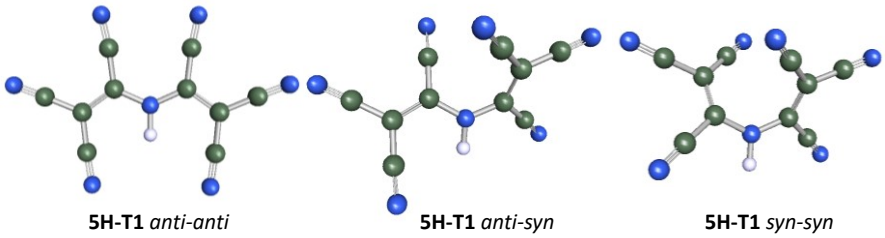
4H-T2 *anti*	**4H-T1** *anti*	**4H-T4** *trans*	**4H-T5** *trans*	**4H-T3** *trans-syn*(H)	**4H-T6** *anti*
0	6.7	15.0	15.2	18.9	32.0

The most stable form for anion **5** is the *anti-anti* conformation. The most stable acid form is **T1**, i.e., the proton attached to the central nitrogen atom. Again, three different conformers (*anti-anti*, *anti-syn*, *syn-syn*) for anion and **4H-T1** (Figure S5), and four different conformers/isomers for other protonated forms can be envisaged. Tautomer **T3**, the CH-acid, has again many possibilities to rotate about C-C bond. 8 different conformers are calculated for **T3** tautomer, *trans-anti-syn*(H) is the most stable form (Table S2).

While anion **4** is fully planar molecule, then anion **5** is not planar. Each TCNV group is planar, the C-N-C angles and the angles between two planes formed from each TCNV group's nitrogen atoms, are the higher the more sterically congested the molecule is (Figure 11).



	5 *anti-anti*	**5** *anti-syn*	**5** *syn-syn*
< TCNV planes [°]	45.3	57.8	62.6
< C-N-C [°]	125.8	126.5	129.5
Δ*G* [kcal/mol]	0	1.8	4.2



	5H-T1 *anti-anti*	**5H-T1** *anti-syn*	**5H-T1** *syn-syn*
< TCNV planes [°]	4.3	53.4	51.1
< C-N-C [°]	131.5	127.8	130.1
Δ*G* [kcal/mol]	0	1.2	3.9

Figure S5. Geometries of three different conformers of anion **5**. The angle between planes composed with N atoms of TCNV groups and bent between C-N-C atoms are presented. The tautomer **T1** as the most stable acid form with the same parameters are brought.

Table S2. Δ*G* values (kcal/mol) of the most stable conformers of different tautomers for compound **5H**, relative to the **5H-T1** *anti-anti* conformer at BP86/def-TZVP level.

5H-T1 *anti-anti*	**5H-T5** *trans-anti*	**5H-T4** *trans-anti*	**5H-T3** *trans-anti-syn*(H)	**5H-T6** *anti-anti*
0	9.1	10.1	14.3	24.8

1.3.3. Central atom C

Replacement of one CN group in cyanoform **6H** with one TCNV group leads to a long-known pentacyanopropene **7H** (Figure S6). The anion **7** and **T6** tautomer of the neutral acid is practically planar (H is bent out of plane 16°). Tautomer **T2** (also **T4** and **T5**) is generally planar, the protonated CN group slightly bent (9–10°) and N-H bond bent out of plane (53°). Tautomer **7H-T3** has stable *syn*(H) and *anti*(H) forms, but the *eclipsed*(H) form is not computationally achievable.

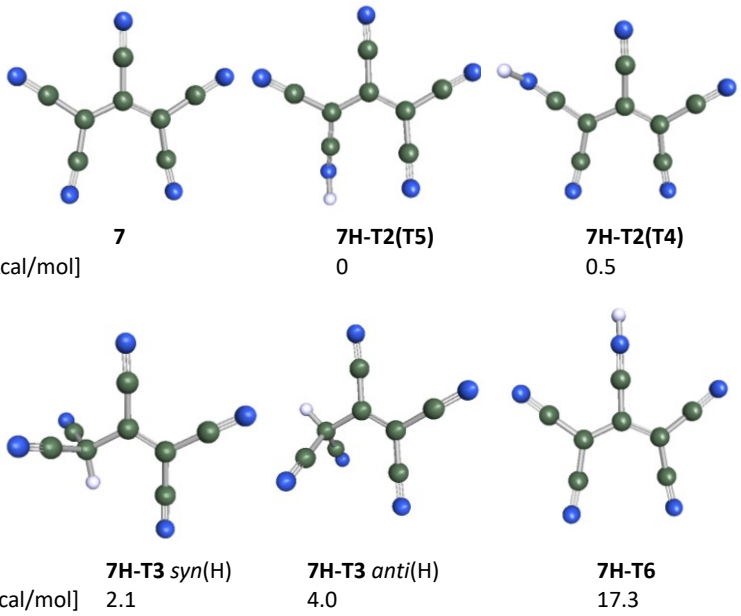


Figure S6. Geometries of **7** and its conjugate acids with their Δ*G* values with respect to the most stable **T2**(**T5**) tautomer.

Second replacement of CN group with TCNV group leads to an anion **8** (Figure S7). Similarly, to N-centered **5**, placing CN group downwards, *syn-syn*, *syn-anti*, and *anti-anti* conformers can be envisaged. Differently from **5**, not an *anti-anti* conformer but the *anti-syn* conformer has the lowest energy while the *anti-anti* form is the least stable one, however, the differences are minor. The torsion angle between TCNV groups (measured as an angle between the planes composed of N atom of TCNV group, < TCNV group) is not consistent with the stability. **8H-T2** tautomer with *anti-syn* conformation is the most stable acid form. The plane using three C atoms around central atom C has been composed and the distance of the central atom C from the plane has been measured (d C-CCC plane), which shows the planarity of the central part of the structure. We can see that the central part is practically planar.

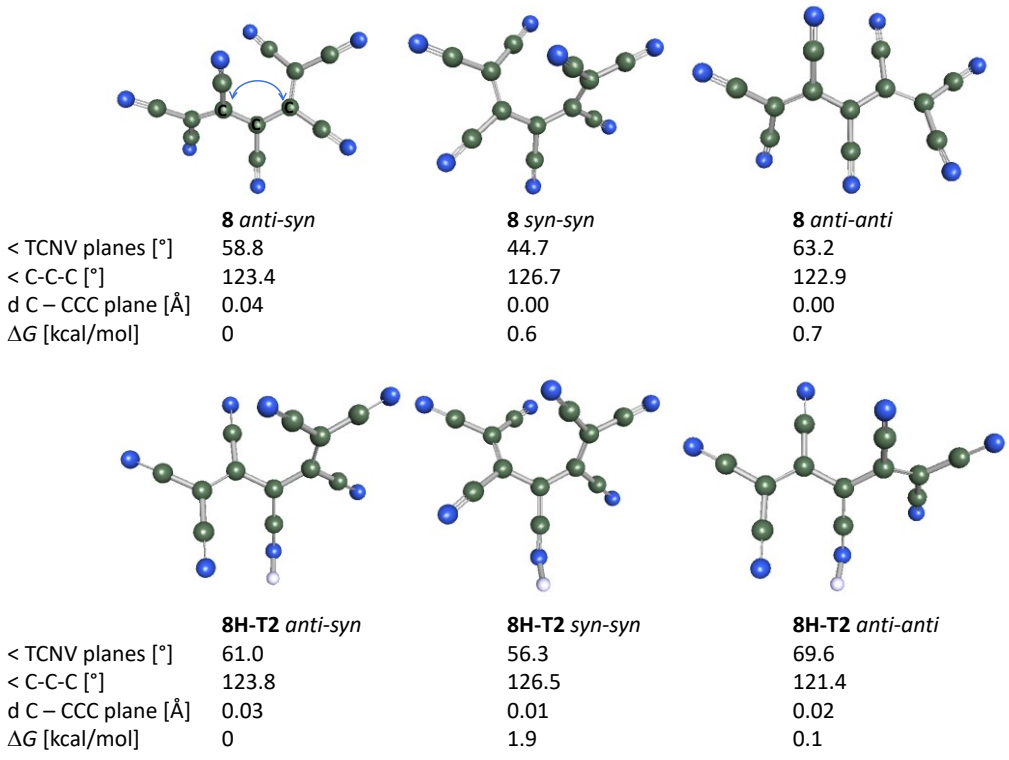


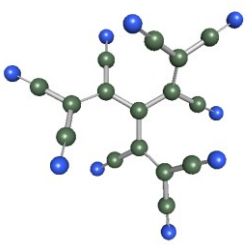
Figure S7. Different conformers of anion **8** and acid form **8H-T2**.

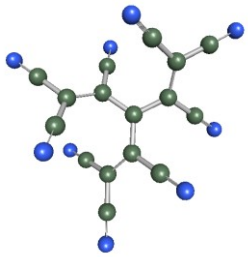
In Table S3 the stability of tautomers of the most stable conformers are available. The differences between different tautomers become smaller compared to the above presented compounds the more TCNV groups the compound incorporates.

Table S3. Δ*G* values (kcal/mol) of the most stable conformers of different tautomers for compound **8H**, relative to the **8H-T2** *anti-syn* conformer at BP86/def-TZVP level.

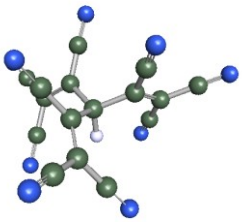
8H-T2 *anti-syn*	**8H-T5** *trans-syn*	**8H-T4** *trans-syn*	**8H-T1** *anti-syn*	**8H-T3** *trans-syn-syn*(H)	**8H-T6** *anti-syn*
0	1.5	2.6	4.0	4.4	16.2

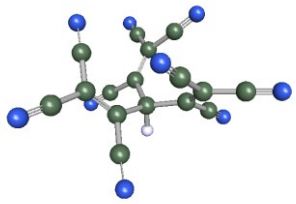
The third replacement of CN group by TCNV group gives the compound **9** with altogether 9 CN groups (Figure S8). In the case of all C-centered anions, also in this case, the central atom C is practically on the same plane as its neighboring C-atoms, therefore, two different anions can be envisaged, the lower energy symmetrical and 2.0 kcal/mol higher energy asymmetrical.





	9 *symmetrical*	**9** *asymmetrical*
< C-C-C [°]	119.9	118.7
	119.9	118.8
	119.9	122.6
d C – CCC plane [Å]	0.05	0.02
Δ*G* [kcal/mol]	0	2.0





	9H-T1 *anti-anti-anti*	**9H-T1** *syn-syn-syn*
< C-C-C [°]	112.0	115.4
	112.1	115.5
	111.9	115.5
d C – CCC plane [Å]	0.44	0.33
Δ*G* [kcal/mol]	0	8.3

Figure S8. Anions **9** with its two conformers and the most stable conjugate acid forms **9H-T1**.

The most stable acid form, **T1**, is slightly more tetrahedron-like, with smaller C-C angle and seemingly higher distance of the central atom from the plane composed its neighbouring C-atoms. The stability of different tautomers shows that **T1, T4** and **T5** tautomers have similar energies (Table S4) and very close GA values (see Table S9). **T6** tautomer comes also energetically closer to other tautomers.

Table S4. ΔG values (kcal/mol) of the most stable conformers of different tautomers for compound **9H**, relative to the **9H-T1** *anti-anti-anti* conformer at BP86/def-TZVP level.

9H-T1 *symmetrical anti-anti-anti*	**9H-T4** *symmetrical trans-anti-anti*	**9H-T5** *symmetrical trans-anti-anti*	**9H-T3** *symmetrical trans-anti-anti- syn*(H)	**9H-T6** *symmetrical anti-anti-anti*
0	1.7	3.0	7.9	13.3

1.3.4. Central atom B

T1 and **T3** tautomers of any boron containing compounds were not achievable computationally, resulting trivalent boron compounds.

Tetracyanoborate, a tetrahedral anion (Figure 7 in the main text), can be replaced with up to four TCNV groups while the configuration stays close to tetrahedron. The angles between bulky TCNV groups, depending on their conformation, are generally somewhat higher compared to the angles between CN groups.

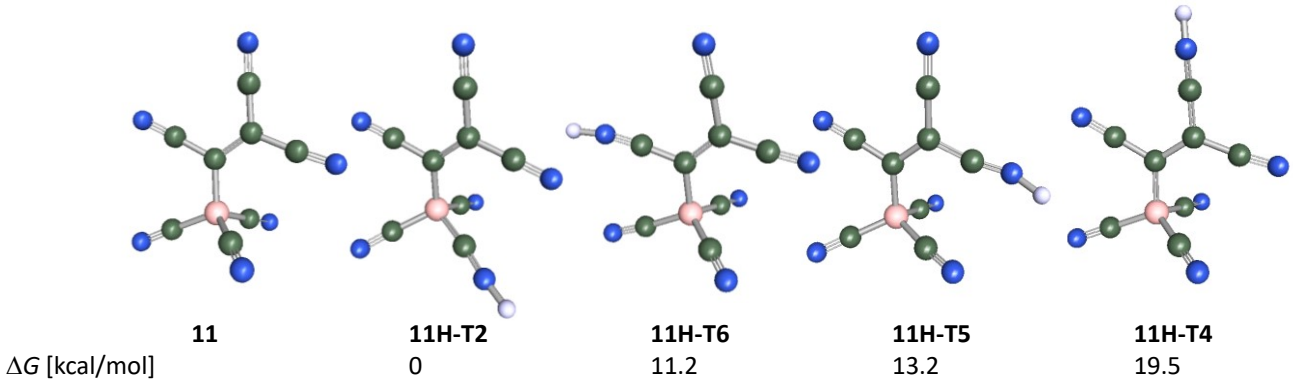


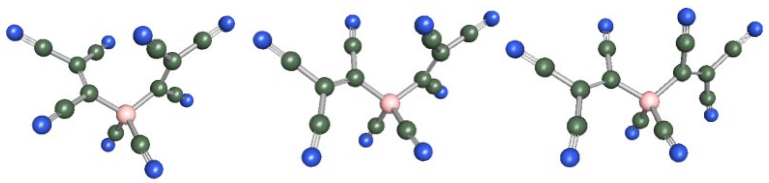
Figure S9. Anion **11** and its different tautomers of conjugate acids.

The most stable tautomer of acid **11H** (Figure S9) is the **T2** tautomer. Three different **T2** tautomers were calculated for each conformation. Differently from O-, N- and C-centered acids, **T6** tautomer is more stable than **T4** and **T5** tauromers.

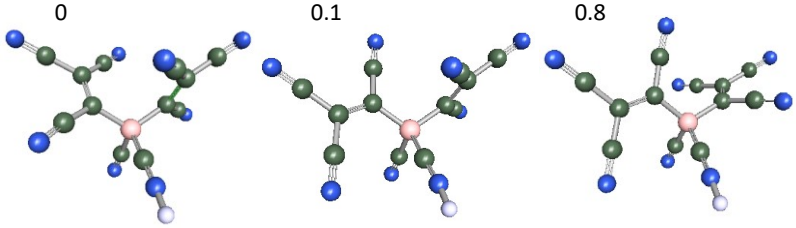
The second replacement of the CN group with the TCNV group leads to an anion (**12**) where three different conformers can be envisaged (Figure S10). Differently from **5**, where *anti-anti*, and from **8**, where *anti-syn* were the most stable conformers, in the case of **12**, most probably because of an additional repulsion from CN groups, the *syn-syn* conformer is the most stable form. Very close is the *anti-syn* conformer in its stability. Two different **T2** tautomers were calculated for each anion, whereas the *anti-syn* form gave the lowest GA value because its protonated form has the highest stability. Again, as shown in Figure 5 in the main text and Table S5, **T6** tautomers are close to **T5** tautomers in their stability. To compare the structures with anions whose central atoms are N (**5**) and C (**8**) atoms, we can see that the C-X-C angle has the smallest value. This comes from the tetrahedral configuration of borates. For anions **5** and **8**, these angles have very similar values being in the range of 123–130 degrees, being the smallest for *anti-anti* conformers and the largest for *syn-syn* conformers.

Table S5. ΔG values (kcal/mol) of the most stable conformers of different tautomers for compound **12H**, relative to the **12H-T2** *anti-syn* conformer at BP86/def-TZVP level.

12H-T2 *anti-syn*	**12H-T6** *syn-anti*	**12H-T5** *trans-syn*	**12H-T4** *trans-syn*
0	10.5	13.2	17.6



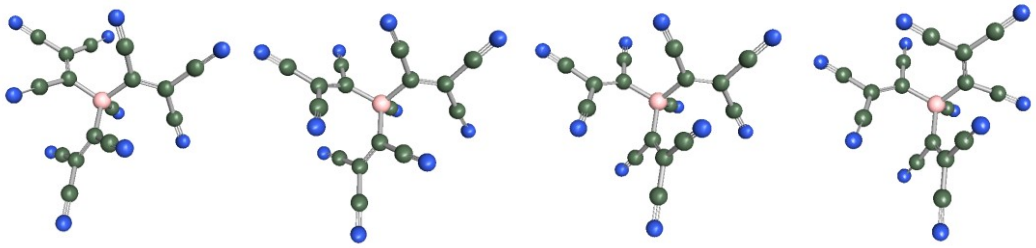
	12 *syn-syn*	**12** *anti-syn*	**12** *anti-anti*
< TCNV planes [°]	77.1	69.9	65.5
< C-B-C [°]	113.3	111.0	109.3
Δ*G* [kcal/mol]	0	0.1	0.8



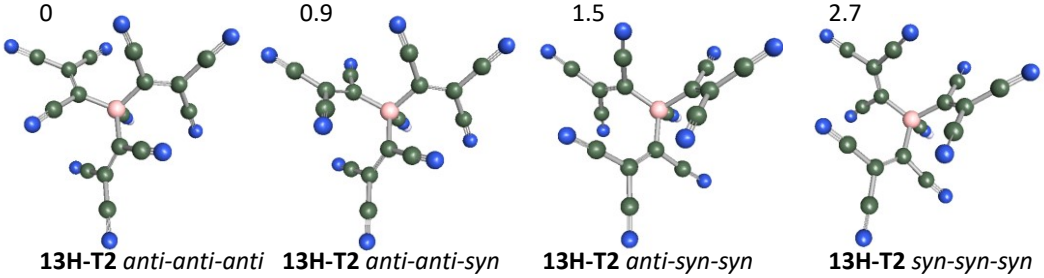
	12H-T2 *syn-syn*	**12H-T2** *anti-syn*	**12H-T2** *anti-anti*
< TCNV planes [°]	82.0	78.5	71.1
< C-B-C [°]	115.9	112.4	113.3
Δ*G* [kcal/mol]	1.1	0	1.1

Figure S10. Three conformers of anion **12** and acid **12H-T2** with their Δ*G* values. The angle between TCNV planes and C-B-C atoms is indicated.

The third replacement of the CN group with the TCNV group gives large-sized anion **13** with four different conformers. Their stability is not too different; however, the most congested *syn-syn-syn* form is the least stable. *Anti-anti-anti* **13H-T2** is the most stable acid form, leaving the second stable **T6** tautomer behind more than 10 kcal/mol (Table S6).



	13 *anti-anti-anti symmetrical*	**13** *anti-anti-syn*	**13** *anti-syn-syn*	**13** *syn-syn-syn symmetrical*
< C-B-C [°]	109.9	108.8	109.0	113.2
	109.9	111.3	112.0	113.4
	109.9	112.4	115.1	113.4
Δ*G* [kcal/mol]	0	0.9	1.5	2.7



	13H-T2 *anti-anti-anti symmetrical*	**13H-T2** *anti-anti-syn*	**13H-T2** *anti-syn-syn*	**13H-T2** *syn-syn-syn symmetrical*
< C-B-C [°]	111.1	114.7	110.2	115.2
	111.4	112.3	113.4	115.1
	111.5	110.4	117.0	115.0
Δ*G* [kcal/mol]	0	0.5	1.1	0.9

Figure S11. Different conformers of anion **13** and its Δ*G* values compared to the most stable, the least congested symmetrical *anti-anti-anti* conformer.

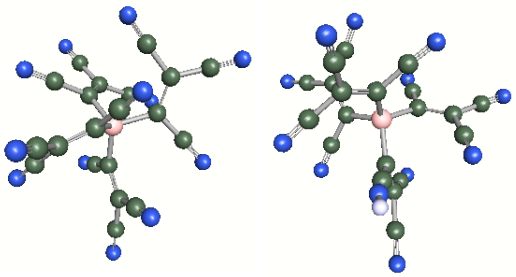
Table S6. ΔG values (kcal/mol) of the most stable conformers of different tautomers for compound **13H**, relative to the **13H-T2** *anti-anti-anti* conformer at BP86/def-TZVP level.

13H-T2	**13H-T5**	**13H-T6**	**13H-T4**
anti-anti-anti	*trans-anti-anti*	*anti-anti-anti*	*trans-anti-anti*
0	13.0	14.3	19.5

The fourth replacement of the CN group with the TCNV group is the most interesting (Figure S12). The most basic site, a single CN group, is now missing. Since no specific configurations for anion could be envisaged, the program COSMOconf was used to find the most stable conformers for anion. Then, four of the most stable anion conformers were chosen, and further calculations were carried out with these. GA values for all the protonation sites in the case of **T4**, **T5,** and **T6** tautomers were calculated. The most stable form is, interestingly, the **T6** tautomer (Table S7).

Table S7. ΔG values (kcal/mol) of the most stable conformers of different tautomers for compound **14H**, relative to the **14H-T6** conformer at BP86/def-TZVP level.

14H-T6	**14H-T5**	**14H-T4**
0	4.0	4.7



	14	**14H-T6**
< C-B-C [°]	109.2	108.2
	109.2	110.3
	109.6	110.4
	109.7	111.4
< H-N-C [°]		172.1

Figure S12. The most stable conformers of anion **14** and its most stable acid form, tautomer **T6**.

1.3.5. Additional acids

Anions of CN^- (**15**) and $TCNV^-$ (**16**) were included in this work for comparison. HCN and HNC are stick-like, and the proton is not bent. Protonated TCNV anion forms interesting structures during optimization (Figure S13); different tautomers exhibit huge instability compared to the most stable acid form.

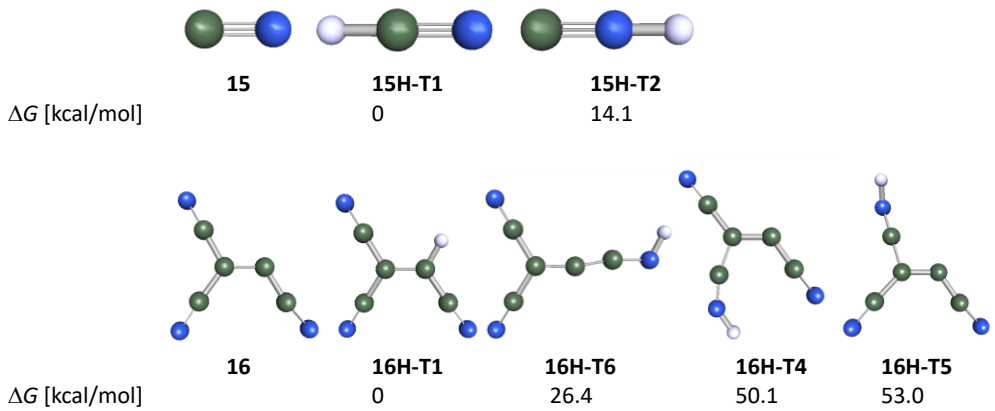


Figure S13. Geometries and ΔG values of CN^- and $TCNV^-$ anions and their acid forms.

Champions in acidity, carborane and dodecaborate acids were included in this work. Only the fully cyanated molecules were studied. As seen from Figure S14, the most stable neutral form of dodecaborate is the one where both protons are as far as possible from each other. The most stable neutral form for carborane acid is the proton attached to the CN group utmost the C-atom of the carborane cage (12 vertex).

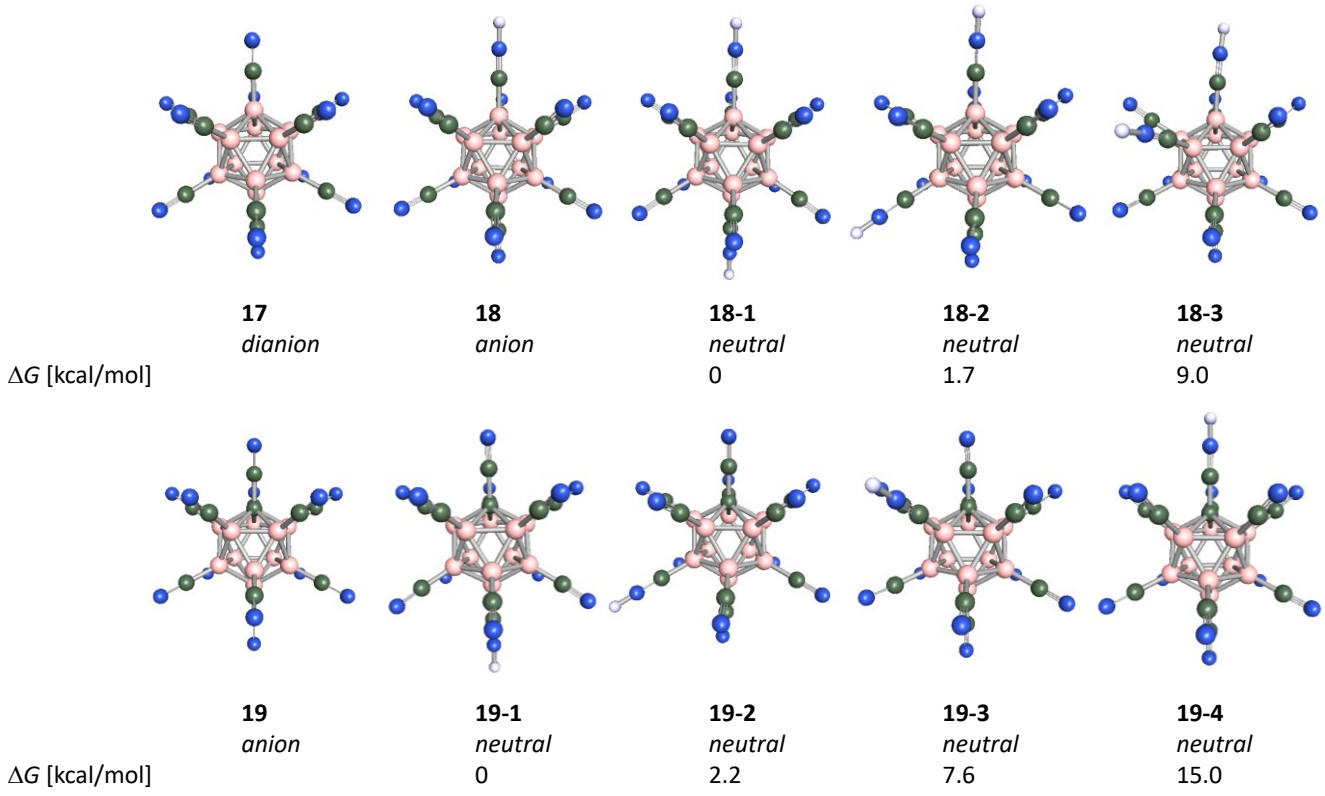


Figure S14. Geometries of dodecaborate dianion **17** and carborane **19** and their protonated forms.

Table S8. pK_a values in different solvents used for final results.

	Compound	COSMO-RS pK_a(MeCN) not corrected	COSMO-RS pK_a(MeCN) corrected	COSMO-RS pK_a(DMSO)	pK_a(DMSO) correlation	pK_a(DMSO) correlation	AVERAGE pK_a(DMSO)	COSMO-RS pK_a(H_2O)	pK_a(DCE) correlation	pK_a(DCE) absolute
		A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**
1H	[CN-O]H	22.0	24.2	10.6	12.1	12.8	12.4	4.8	14.7	59.7
2H	[O-TCNV]H	2.9	5.1	-5.1	-7.4	-6.7	-7.0	-3.2	-6.6	38.4
3H	[$(CN)_2$N]H	10.3	12.5	0.9	0.2	0.9	0.5	0.0	1.7	46.7
4H	[CN-N-TCNV]H	3.6	5.7	-4.9	-6.7	-6.0	-6.3	-2.7	-5.8	39.2
5H	[N-$TCNV_2$]H	-1.0	1.2	-8.6	-11.4	-10.6	-11.0	-4.5	-10.9	34.1
6H	[$(CN)_3$C]H	2.8	4.9	-5.4	-7.6	-6.8	-7.2	-3.6	-6.8	38.2
7H	[$(CN)_2$-C-TCNV]H	-4.6	-2.4	-11.2	-15.1	-14.3	-14.7	-7.3	-15.0	30.0
8H	[CN-C-$TCNV_2$]H	-7.3	-5.2	-13.3	-17.9	-17.1	-17.5	-8.7	-18.0	27.0
9H	[C-$TCNV_3$]H	-9.7	-7.6	-15.0	-20.3	-19.6	-20.0	-10.0	-20.7	24.3
10H	[$(CN)_4$B]H	-5.6	-3.5	-11.5	-16.1	-15.4	-15.8	-7.8	-16.1	28.9
11H	[$(CN)_3$-B-TCNV]H	-6.2	-4.1	-12.0	-16.8	-16.0	-16.4	-8.0	-16.8	28.2
12H	[$(CN)_2$-B-$TCNV_2$]H	-7.1	-4.9	-12.6	-17.6	-16.9	-17.2	-8.3	-17.7	27.3
13H	[CN-B-$TCNV_3$]H	-8.0	-5.9	-13.3	-18.6	-17.9	-18.2	-8.8	-18.8	26.2
14H	[B-$TCNV_4$]H	-15.0	-12.9	-18.6	-25.7	-25.0	-25.3	-13.0	-26.6	18.4
15H	HCN	26.2	28.4	14.6	16.4	17.1	16.8	8.6	19.4	64.4
16H	$C(CN)_2$=CH(CN)	27.4	29.7	13.2	17.7	18.4	18.1	11.6	20.8	65.8
17H	$[B_{12}(CN)_{12}]H^-$	-10.2	-8.1	-14.9	-20.8	-20.1	-20.4	-11.3	-21.2	23.8
18H	$[B_{12}(CN)_{12}]H_2$	-13.5	-11.4	-17.8	-24.1	-23.4	-23.8	-11.8	-24.9	20.1
19H	$[CB_{11}(CN)_{12}]$H	-16.3	-14.2	-19.8	-27.1	-26.4	-26.7	-13.3	-28.1	16.9

A: COSMO-RS pK_a(MeCN) values obtained from the calculations according to the .cosmo files available in DataDoi data repository. Different tautomers and conformers are taken into account.
B: COSMO-RS pK_a(MeCN) values that are corrected according to Eq 4 in the main text.
C: COSMO-RS pK_a(DMSO) values obtained from the calculations according to the .cosmo files available in DataDoi data repository.
D: pK_a(DMSO) values that are obtained from the correlation from corrected pK_a(MeCN) values (column B) using the equation from Ref [42] in the main text.
E: pK_a(DMSO) values that are obtained from the correlation from corrected pK_a(MeCN) values (column B) using the equation from Ref [34] in the main text.
F: Final assigned pK_a(DMSO) values that are obtained by averaging pK_a(DMSO) values from columns D and E.
G: COSMO-RS pK_a(H_2O) values obtained from the calculations according to the .cosmo files available in DataDoi data repository. The values are not corrected.
H: Relative pK_a(DCE) values that are obtained from the correlation from corrected pK_a(MeCN) values (column B) using the equation from Ref [3] in the main text.
G: Absolute pK_a(DCE) values according to the Ref [37] in the main text. All these values are 45.0 units higher than the values in column H.

Table S9. The total molecular energies, PA and GA values, and a number of imaginary frequencies (N imag) of the studied molecules. When different conformers are named, the first group in the row of the names is always the protonated TCNV group, and counting continues clockwise, or the position of the proton is specifically noted. A single CN group or proton, in the case of **T1** and **T2**, is generally facing downwards or backward. Conformation of the TCNV group in the case of compounds **9H** and **13H** are determined regarding the C-C-C plane around central atom C or B, respectively; the conformation is decided according to the CN group in 1st position of the TCNV group.

Compound	Basis set	Total energy Ha	Enthalpy Ha	*H* Ha	PA kcal/mol	Chem. Pot. Ha	*G* Ha	GA kcal/mol	N imag
1									
Anion									
	BP86/def-TZVP	-168.207622	0.014630	-168.192992		-0.010231	-168.217852		0
	BP86/def2-TZVPP	-168.214437	0.014653	-168.199784		-0.010202	-168.224639		0
	BP86/def2-TZVPPD	-168.218957	0.014584	-168.204373		-0.010276	-168.229233		0
	B3LYP/def2-TZVPPD	-168.122537	0.015239	-168.107298		-0.001430	-168.123967		0
	B3LYP/6-311+G(d,p)			-168.172144			-168.197063		0
	G4(MP2)			-167.955641			-167.980531		0
	W1RO			-168.200611			-168.225527		0
	CBS-APNO			-168.113344			-168.138159		0
Neutral									
T1	BP86/def-TZVP	-168.716794	0.024878	-168.691916	314.6	-0.002685	-168.719479	308.5	0
T2	BP86/def-TZVP	-168.764542	0.024798	-168.739744	344.6	-0.002388	-168.766930	338.3	0
	BP86/def2-TZVPP	-168.774659	0.024827	-168.749832	346.6	-0.002359	-168.777018	340.3	0
	BP86/def2-TZVPPD	-168.775643	0.024820	-168.750823	344.4	-0.002365	-168.778008	338.1	0
	B3LYP/def2-TZVPPD	-168.678486	0.025321	-168.653165	344.0	-0.001785	-168.680271	342.8	0
	B3LYP/6-311+G(d,p)			-168.713282	341.0		-168.740361	334.6	0
	G4(MP2)			-168.497657	341.6		-168.524743	335.2	0
	W1RO			-168.742541	341.5		-168.769626	335.1	0
	CBS-APNO			-168.655663	341.8		-168.682714	335.4	0
2									
Anion									
	BP86/def-TZVP	-430.226987	0.047818	-430.179169		0.004879	-430.222108		0
	BP86/def2-TZVPP	-430.245433	0.047779	-430.197654		0.004868	-430.240565		0
	BP86/def2-TZVPPD	-430.248071	0.047724	-430.200347		0.004780	-430.243291		0
	B3LYP/def2-TZVPPD	-429.993634	0.049008	-429.944626		0.006489	-429.987145		0
	B3LYP/6-311+G(d,p)			-430.118532			-430.160900		0
	G4(MP2)			-429.535840			-429.578200		0
	W1RO			-430.171189			-430.213701		0
	CBS-APNO			-429.989995			-430.032120		0
Neutral									

T1	BP86/def-TZVP	-430.698883	0.060176	-430.638707	289.8	0.016565	-430.682319	282.5	0
	BP86/def2-TZVPP	-430.720183	0.060251	-430.659932	291.6	0.016697	-430.703486	284.2	0
	BP86/def2-TZVPPD	-430.721855	0.060231	-430.661624	290.9	0.016709	-430.705146	283.5	0
	B3LYP/def2-TZVPPD	-430.468759	0.061838	-430.406921	291.6	0.018721	-430.450038	284.2	0
	B3LYP/6-311+G(d,p)			-430.577397	289.4		-430.620442	282.1	0
	G4(MP2)			-430.002708	294.4		-430.045755	287.1	0
	W1RO			-430.637035	293.8		-430.680197	286.5	0
	CBS-APNO			-430.453922	292.6		-430.49682	285.3	0
T3; eclipsed(H)	BP86/def-TZVP	-430.685699	0.059358	-430.626341	282.1	0.014557	-430.671142	275.5	0
T3; syn(H)	BP86/def-TZVP	-430.686088	0.059539	-430.626549	282.2	0.014566	-430.671522	275.7	0
T3; anti(H)	BP86/def-TZVP	-430.683587	0.058586	-430.625001	281.2	0.016476	-430.667111	273.0	1
T4	BP86/def-TZVP	-430.691937	0.059061	-430.632876	286.2	0.015090	-430.676847	279.1	0
T5	BP86/def-TZVP	-430.691022	0.059076	-430.631946	285.6	0.015018	-430.676004	278.5	0
T6	BP86/def-TZVP	-430.663974	0.057860	-430.606114	269.4	0.012976	-430.650998	262.9	0
3									
Anion									
	BP86/def-TZVP	-240.607141	0.025478	-240.581663		-0.006791	-240.613933		0
	BP86/def2-TZVPP	-240.618830	0.025484	-240.593346		-0.006740	-240.625570		0
	BP86/def2-TZVPPD	-240.621254	0.025456	-240.595798		-0.006778	-240.628032		0
	B3LYP/def2-TZVPPD	-240.474743	0.026101	-240.448642		-0.005964	-240.480707		0
	B3LYP/6-311+G(d,p)			-240.548045			-240.580080		0
	G4(MP2)			-240.216648			-240.248658		0
	W1RO			-240.568517			-240.600555		0
	CBS-APNO			-240.46843			-240.500308		0
Neutral									
T1	BP86/def-TZVP	-241.101085	0.037495	-241.063590	303.9	0.003874	-241.097211	297.0	0
T2	BP86/def-TZVP	-241.116908		-241.116908	337.3	0.003535	-241.113374	307.1	0
	BP86/def2-TZVPP	-241.131063	0.036729	-241.094334	315.9	0.003631	-241.127432	308.6	0
	BP86/def2-TZVPPD	-241.132002	0.036724	-241.095278	314.9	0.003624	-241.128378	307.7	0
	B3LYP/def2-TZVPPD	-240.984167	0.037589	-240.946578	313.9	0.004685	-240.979482	306.7	0
	B3LYP/6-311+G(d,p)			-241.042429	311.7		-241.075302	304.5	0
	G4(MP2)			-240.709896	311.0		-240.742776	303.8	0
	W1RO			-241.061506	310.8		-241.094404	303.6	0
	CBS-APNO			-240.961639	311.0		-240.994359	303.7	0
4									
Anion									
anti	BP86/def-TZVP	-502.618281	0.060086	-502.558195		0.012379	-502.605902		0

	BP86/def2-TZVPP	-502.641764	0.060064	-502.581700		0.012401	-502.629363		0
	BP86/def2-TZVPPD	-502.644033	0.060001	-502.584032		0.012292	-502.631741		0
	B3LYP/def2-TZVPPD	-502.338368	0.061590	-502.276778		0.014455	-502.323913		0
	B3LYP/6-311+G(d,p)			-502.486274			-502.533246		0
	G4(MP2)			-501.791892			-501.838878		0
	W1RO			-502.532800			-502.579916		0
	CBS-APNO			-502.339803			-502.386434		0
syn	BP86/def-TZVP	-502.613592	0.060053	-502.553539		0.012192	-502.601400		0
	BP86/def2-TZVPP	-502.636604	0.060022	-502.576582		0.012236	-502.624368		0
Neutral									
T1; syn	BP86/def-TZVP	-503.077630	0.072579	-503.005051	284.8	0.023085	-503.054544	278.1	0
T1; anti	BP86/def-TZVP	-503.083250	0.072541	-503.010709	285.4	0.023885	-503.059364	278.3	0
T2; anti	BP86/def-TZVP	-503.092361	0.071365	-503.020996	291.9	0.022293	-503.070068	285.0	0
	BP86/def2-TZVPP	-503.118123	0.071368	-503.046755	293.3	0.022373	-503.095750	286.4	0
	BP86/def2-TZVPPD	-503.119703	0.071330	-503.048373	292.9	0.022281	-503.097422	285.9	0
	B3LYP/def2-TZVPPD	-502.813497	0.073115	-502.740382	292.4	0.024645	-502.788852	285.5	0
	B3LYP/6-311+G(d,p)			-502.946737	290.4		-502.995025	283.5	0
	G4(MP2)			-502.252907	290.8		-502.301252	283.9	0
	W1RO			-502.993228	290.4		-503.041704	283.5	0
	CBS-APNO			-502.799239	289.8		-502.847250	282.9	0
T2; syn	BP86/def-TZVP	-503.090845	0.071325	-503.019520	293.9	0.022419	-503.068426	286.8	0
	BP86/def2-TZVPP	-503.116373	0.071347	-503.045026	295.4	0.022545	-503.093828	288.3	0
T3; trans, eclipsed(H)	BP86/def-TZVP	-503.061094	0.071521	-502.989573	272.2	0.022088	-503.039006	265.5	0
T3; trans, syn(H)	BP86/def-TZVP	-503.062100	0.071635	-502.990465	272.7	0.022163	-503.039937	266.1	0
T3; cis, anti(H)	BP86/def-TZVP	-503.057950	0.071583	-502.986367	273.1	0.022316	-503.035634	266.2	0
T3; cis, syn(H)	BP86/def-TZVP	-503.060834	0.071613	-502.989221	274.9	0.022209	-503.038625	268.1	0
T4; trans	BP86/def-TZVP	-503.068630	0.071146	-502.997484	277.1	0.022537	-503.046093	269.9	0
T4; cis	BP86/def-TZVP	-503.064892	0.071039	-502.993853	277.8	0.022164	-503.042729	270.7	0
T5; trans	BP86/def-TZVP	-503.068128	0.071142	-502.996986	276.8	0.022344	-503.045784	269.8	0
T5; cis	BP86/def-TZVP	-503.067114	0.071113	-502.996001	279.1	0.022738	-503.044376	271.7	0
T6; anti	BP86/def-TZVP	-503.039063	0.070006	-502.969057	259.3	0.019915	-503.019148	253.0	0
T6; syn	BP86/def-TZVP	-503.034477	0.070179	-502.964298	259.2	0.019713	-503.014764	253.1	0
5									
Anion									
Anion; anti-syn (syn facing forward)	BP86/def-TZVP	-764.601870	0.094724	-764.507146		0.03208581	-764.569784		0
Anion; anti-syn (syn facing backward)	BP86/def-TZVP	-764.601863	0.094718	-764.507145		0.03207300	-764.569790		0
	BP86/def2-TZVPP	-764.636463	0.094656	-764.541807		0.03207300	-764.604390		0
anti-anti	BP86/def-TZVP	-764.605066	0.094637	-764.510429		0.03244700	-764.572619		0

	BP86/def2-TZVPP	-764.639837	0.094581	-764.545256		0.03166500	-764.608172		0
	BP86/def2-TZVPPD	-764.642582	0.094465	-764.548117		0.03100900	-764.611573		0
	B3LYP/def2-TZVPPD	-764.177664	0.097000	-764.080664		0.03470100	-764.142963		0
	B3LYP/6-311+G(d,p)			-764.400802			-764.462556		0
	G4(MP2)			-763.345822			-763.407662		0
	CBS-APNO			-764.190708			-764.252022		0
syn-syn	BP86/def-TZVP	-764.598170	0.094726	-764.503444		0.03228400	-764.565886		0
Neutral									
T1; anti-syn (syn facing forward)	BP86/def-TZVP	-765.051942	0.107391	-764.944551	276.0	0.04410500	-765.007837	268.6	0
T1; anti-syn (syn facing backward)	BP86/def-TZVP	-765.051928	0.107361	-764.944567	276.0	0.04404181	-765.007886	268.6	0
	BP86/def2-TZVPP	-765.087543	0.107302	-764.980241	276.6	0.04403000	-765.043513	269.3	0
T1; syn-syn	BP86/def-TZVP	-765.048189	0.107416	-764.940773	275.9	0.04460700	-765.003582	268.4	0
T1; anti-anti	BP86/def-TZVP	-765.056284	0.107464	-764.948820	276.6	0.04369700	-765.012587	269.8	0
	BP86/def2-TZVPP	-765.092233	0.107387	-764.984846	277.3	0.04358200	-765.048651	270.1	0
	BP86/def2-TZVPPD	-765.094552	0.107236	-764.987316	277.1	0.04227200	-765.052280	270.3	0
	B3LYP/def2-TZVPPD	-764.631166	0.110206	-764.520960	277.8	0.04687100	-764.584295	270.7	0
	B3LYP/6-311+G(d,p)			-764.838918	276.4		-764.901472	269.1	0
	G4(MP2)			-763.792555	281.8		-763.855306	274.6	0
	CBS-APNO			-764.63221	278.5		-764.694763	271.5	0
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	-765.025965	0.106032	-764.919933	260.5	0.04185933	-764.984105	253.7	0
T3; cis-anti, syn(H)	BP86/def-TZVP	-765.025564	0.106185	-764.919379	260.2	0.04065200	-764.984912	254.2	0
T3; trans-anti, syn(H)	BP86/def-TZVP	-765.030874	0.106238	-764.924636	261.4	0.04114708	-764.989727	255.5	0
T3; trans-anti, eclipsed(H)	BP86/def-TZVP	-765.029303	0.106140	-764.923163	260.5	0.04102600	-764.988277	254.6	0
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	-765.025547	0.106099	-764.919448	262.5	0.04274000	-764.982807	255.3	0
T3; cis-syn, syn(H)	BP86/def-TZVP	-765.023788	0.106339	-764.917449	261.3	0.04118100	-764.982607	255.2	0
T3; trans-syn, syn(H)	BP86/def-TZVP	-765.028440	0.106418	-764.922022	261.8	0.04126600	-764.987174	255.6	0
T3; trans-syn, eclipsed(H)	BP86/def-TZVP	-765.029077	0.106315	-764.922762	262.3	0.04156800	-764.987509	255.8	0
T4; cis-anti	BP86/def-TZVP	-765.034108	0.105774	-764.928334	265.8	0.04181363	-764.992295	258.9	0
T4; trans-anti	BP86/def-TZVP	-765.038000	0.105731	-764.932269	266.2	0.04156986	-764.996430	259.7	0
T4; cis-syn	BP86/def-TZVP	-765.033990	0.105858	-764.928132	268.0	0.04209200	-764.991898	261.0	0
T4; trans-syn	BP86/def-TZVP	-765.037230	0.105928	-764.931302	267.6	0.04198600	-764.995244	260.7	0
T5; trans-anti	BP86/def-TZVP	-765.039415	0.105696	-764.933719	267.1	0.04126900	-764.998146	260.7	0
T5; cis-syn	BP86/def-TZVP	-765.030109	0.105821	-764.924288	265.6	0.04059900	-764.989510	259.5	0
T5; trans-syn	BP86/def-TZVP	-765.035593	0.105876	-764.929717	266.6	0.04164700	-764.993946	259.9	0
T5; cis-anti	BP86/def-TZVP	-765.031063	0.105717	-764.925346	263.9	0.04159800	-764.989465	257.1	0
T6; anti-anti	BP86/def-TZVP	-765.012987	0.104621	-764.908366	251.2	0.03991400	-764.973073	245.0	0
T6; syn-syn	BP86/def-TZVP	-765.004797	0.104861	-764.899936	250.3	0.04024200	-764.964555	243.9	0
T6; anti-syn	BP86/def-TZVP	-765.009335	0.104766	-764.904569	250.9	0.04059800	-764.968737	244.1	0
T6; syn-anti	BP86/def-TZVP	-765.007737	0.104857	-764.902880	249.8	0.03981100	-764.967926	243.6	0

6									
Anion									
	BP86/def-TZVP	-316.838101	0.037123	-316.800978		-0.000673	-316.838774		0
	BP86/def2-TZVPP	-316.851152	0.037055	-316.814097		-0.000747	-316.851899		0
	BP86/def2-TZVPPD	-316.853112	0.037007	-316.816105		-0.000834	-316.853946		0
	B3LYP/def2-TZVPPD	-316.663083	0.037914	-316.625169		0.000340	-316.662743		0
	B3LYP/6-311+G(d,p)			-316.760517			-316.797325		0
	G4(MP2)			-316.317077			-316.353858		0
	W1RO			-316.784822			-316.821714		0
	CBS-APNO			-316.662846			-316.699558		0
Neutral									
T1	BP86/def-TZVP	-317.316257	0.048770	-317.267487	294.2	0.010067	-317.306190	287.0	0
T2	BP86/def-TZVP	-317.317464	0.048394	-317.269070	295.2	0.009899	-317.307564	287.9	0
	BP86/def2-TZVPP	-317.332801	0.048398	-317.284403	296.6	0.009906	-317.322895	289.3	0
	BP86/def2-TZVPPD	-317.333837	0.048380	-317.285457	296.0	0.009873	-317.323964	288.7	0
	B3LYP/def2-TZVPPD	-317.142341	0.049588	-317.092753	294.9	0.011412	-317.130929	287.5	0
	B3LYP/6-311+G(d,p)			-317.225116	293.0		-317.263178	286.0	0
	G4(MP2)			-316.782681	293.6		-316.820796	286.7	0
	W1RO			-317.249515	293.1		-317.287697	286.1	0
	CBS-APNO			-317.127541	293.1		-317.165395	286.0	0
7									
Anion									
	BP86/def-TZVP	-578.840073	0.071969	-578.768104		0.018458	-578.821616		0
	BP86/def2-TZVPP	-578.865138	0.071856	-578.793282		0.018561	-578.846577		0
	BP86/def2-TZVPPD	-578.867407	0.071772	-578.795635		0.017646	-578.849761		0
	B3LYP/def2-TZVPPD	-578.516890	0.073615	-578.443275		0.020553	-578.496337		0
	B3LYP/6-311+G(d,p)			-578.688752			-578.741177		0
	G4(MP2)			-577.885015			-577.937095		0
	CBS-APNO			-578.528093			-578.579917		0
Neutral									
T3 = T1; anti(H)	BP86/def-TZVP	-579.282082	0.083653	-579.198429	271.5	0.029599	-579.252483	264.1	0
T3 = T1; syn(H)	BP86/def-TZVP	-579.284980	0.083670	-579.201310	273.3	0.029412	-579.255568	266.0	0
T2 = T4	BP86/def-TZVP	-579.287094	0.083051	-579.204043	275.0	0.028951	-579.258142	267.6	0
T2 = T5	BP86/def-TZVP	-579.288599	0.083009	-579.205590	276.0	0.029706	-579.258893	268.1	0
	BP86/def2-TZVPP	-579.315697	0.082957	-579.232740	277.2	0.029635	-579.286062	269.5	0
	BP86/def2-TZVPPD	-579.317462	0.082883	-579.234579	276.9	0.029432	-579.288030	268.7	0
	B3LYP/def2-TZVPPD	-578.965768	0.085023	-578.880745	276.0	0.032331	-578.933437	268.0	0

	B3LYP/6-311+G(d,p)			-579.123607	274.4		-579.175982	266.6	0
	G4(MP2)			-578.321248	275.2		-578.373823	267.8	0
	CBS-APNO			-578.961449	273.4		-579.013592	265.9	0
T6	BP86/def-TZVP	-579.257315	0.082131	-579.175184	256.9	0.026048	-579.231267	250.8	0
8									
Anion									
syn-syn	BP86/def-TZVP	-840.819797	0.106493	-840.713304		0.040279	-840.779518		0
anti-syn	BP86/def-TZVP	-840.820188	0.106488	-840.713700		0.039776	-840.780412		0
	BP86/def2-TZVPP	-840.856841	0.106409	-840.750432		0.039752	-840.817089		0
	BP86/def2-TZVPPD	-840.859815	0.106167	-840.753648		0.038530	-840.821285		0
	B3LYP/def2-TZVPPD	-840.348210	0.108981	-840.239229		0.042792	-840.305418		0
	B3LYP/6-311+G(d,p)			-840.595443			-840.660817		0
	G4(MP2)			-839.434863			-839.500343		0
	CBS-APNO			-840.375867			-840.441015		0
anti-anti	BP86/def-TZVP	-840.818932	0.106470	-840.712462		0.039575	-840.779357		0
	BP86/def2-TZVPP	-840.855634	0.106383	-840.749251		0.039492	-840.816142		0
Neutral									
T1; syn-syn	BP86/def-TZVP	-841.242638	0.118320	-841.124318	259.4	0.049481	-841.193157	253.3	0
T1; anti-anti	BP86/def-TZVP	-841.249249	0.118370	-841.130879	264.0	0.049039	-841.200210	257.8	0
T1; anti-syn = syn-anti	BP86/def-TZVP	-841.247075	0.118447	-841.128628	261.8	0.049382	-841.197693	255.6	0
T2; anti-anti	BP86/def-TZVP	-841.253550	0.117618	-841.135932	267.2	0.049683	-841.203867	260.1	0
	BP86/def2-TZVPP	-841.292416	0.117539	-841.174877	268.6	0.049657	-841.242759	261.4	0
T2; syn-anti	BP86/def-TZVP	-841.253972	0.117674	-841.136298	266.7	0.049923	-841.204049	259.6	0
	BP86/def2-TZVPP	-841.292832	0.117608	-841.175224	268.0	0.049927	-841.242905	260.9	0
	BP86/def2-TZVPPD	-841.295398	0.116396	-841.179002	268.4	0.050723	-841.244675	259.4	1
	B3LYP/def2-TZVPPD	-840.783550	0.120449	-840.663101	267.5	0.052403	-840.731147	260.9	0
	B3LYP/6-311+G(d,p)			-841.016524	265.7		-841.083003	258.6	0
	G4(MP2)			-839.858440	267.3		-839.924998	260.2	0
	CBS-APNO			-840.794097	263.9		-840.860383	256.9	0
T2; syn-syn	BP86/def-TZVP	-841.250505	0.117636	-841.132869	263.3	0.049471	-841.201034	258.2	0
T3; cis-anti, anti(H)	BP86/def-TZVP	-841.240404	0.118230	-841.122174	257.8	0.049580	-841.190824	251.3	0
T3; cis-anti, syn(H)	BP86/def-TZVP	-841.241724	0.118223	-841.123501	258.6	0.048605	-841.193119	252.7	0
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	-841.241562	0.118102	-841.123460	258.6	0.049473	-841.192089	252.1	0
T3; trans-anti, syn(H)	BP86/def-TZVP	-841.245605	0.118323	-841.127282	261.8	0.048582	-841.197023	255.8	0
T3; trans-anti, anti(H)	BP86/def-TZVP	-841.243104	0.118339	-841.124765	260.2	0.049261	-841.193843	253.8	0
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	-841.240368	0.118014	-841.122354	258.2	0.049750	-841.190618	251.7	0
T3; trans-syn, syn(H)	BP86/def-TZVP	-841.245773	0.118340	-841.127433	261.1	0.048742	-841.197031	255.2	0
T3; trans-syn, anti(H)	BP86/def-TZVP	-841.242490	0.118339	-841.124151	259.0	0.049261	-841.193229	252.8	0

T4; cis-anti	BP86/def-TZVP	-841.249331	0.117665	-841.131666	263.8	0.049472	-841.199859	256.9	0
T4; cis-syn	BP86/def-TZVP	-841.250673	0.117681	-841.132992	264.8	0.049969	-841.200704	258.0	0
T4; trans-syn	BP86/def-TZVP	-841.248912	0.117640	-841.131272	263.5	0.048967	-841.199945	257.0	0
T4; trans-anti	BP86/def-TZVP	-841.248112	0.117615	-841.130497	263.8	0.048609	-841.199503	257.4	0
T5; trans-anti	BP86/def-TZVP	-841.250613	0.117564	-841.133049	265.4	0.049516	-841.201097	258.4	0
T5; cis-syn	BP86/def-TZVP	-841.243476	0.117516	-841.125960	260.4	0.048344	-841.195132	254.5	0
T5; cis-anti	BP86/def-TZVP	-841.247755	0.117542	-841.130213	262.8	0.049631	-841.198124	255.8	0
T5; trans-syn	BP86/def-TZVP	-841.251210	0.117606	-841.133604	265.0	0.049605	-841.201605	258.0	0
T6; anti-anti	BP86/def-TZVP	-841.226314	0.116810	-841.109504	250.6	0.048300	-841.178014	243.9	0
T6; anti-syn	BP86/def-TZVP	-841.226771	0.116831	-841.109940	250.1	0.048584	-841.178187	243.3	0
T6; syn-anti	BP86/def-TZVP	-841.225384	0.116778	-841.108606	249.3	0.047876	-841.177508	242.9	0
T6; syn-syn	BP86/def-TZVP	-841.226830	0.116809	-841.110021	250.4	0.048811	-841.178019	243.8	0
9									
Anion									
symmetrical	BP86/def-TZVP	-1102.795471	0.141117	-1102.654354		0.060374	-1102.735097		0
	BP86/def2-TZVPP	-1102.843579	0.141008	-1102.702571		0.060361	-1102.783218		0
	BP86/def2-TZVPPD	-1102.847365	0.137131	-1102.710234		0.061533	-1102.785832		3
	B3LYP/def2-TZVPPD	-1102.175386	0.142990	-1102.032396		0.063331	-1102.112055		1
	B3LYP/6-311+G(d,p)			-1102.498180			-1102.577184		0
	G4(MP2)			-1100.985095			-1101.064353		0
asymmetrical	BP86/def-TZVP	-1102.792184	0.141033	-1102.651151		0.060328	-1102.731856		0
	BP86/def2-TZVPP	-1102.840299	0.140916	-1102.699383		0.060307	-1102.779992		0
Neutral									
T1; asymmetrical, anti-syn-syn; H facing backward	BP86/def-TZVP	-1103.206239	0.153113	-1103.053126	253.7	0.070041	-1103.136198	247.4	0
T1; symmetrical, syn-syn-syn; H facing backward	BP86/def-TZVP	-1103.201043	0.153094	-1103.047949	248.5	0.069752	-1103.131292	242.3	0
T1; symmetrical, anti-anti-anti; H facing backward	BP86/def-TZVP	-1103.212726	0.153173	-1103.059553	255.7	0.068203	-1103.144523	250.6	0
	BP86/def2-TZVPP	-1103.260230	0.152924	-1103.107306	255.5	0.067924	-1103.192306	250.4	0
	BP86/def2-TZVPPD	-1103.263562	0.146096	-1103.117466	255.5	0.071837	-1103.191725	248.4	5
	B3LYP/def2-TZVPPD	-1102.597219	0.153142	-1102.444077	258.3	0.076612	-1102.520607	250.1	3
	B3LYP/6-311+G(d,p)			-1102.906469	257.7		-1102.989190	252.3	0
	G4(MP2)			-1101.404301	264.5		-1101.487830	259.5	0
T1; asymmetrical, anti-anti-syn; H facing backward	BP86/def-TZVP	-1103.209141	0.153139	-1103.056002	255.5	0.069185	-1103.139956	249.8	0
T3; trans-syn-syn, eclipsed(H)	BP86/def-TZVP	-1103.199969	0.152604	-1103.047365	248.1	0.069687	-1103.130282	241.7	0
T3; trans-syn-syn, anti(H)	BP86/def-TZVP	-1103.196756	0.152712	-1103.044044	246.0	0.069340	-1103.127416	241.9	0
T3; trans-syn-syn, syn(H)	BP86/def-TZVP	-1103.198806	0.152859	-1103.045947	247.2	0.069096	-1103.129710	243.4	0
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	-1103.200018	0.152818	-1103.047200	250.0	0.068820	-1103.131198	244.3	0
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	-1103.198490	0.152737	-1103.045753	249.1	0.070263	-1103.128227	242.4	0
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	-1103.200162	0.152651	-1103.047511	250.2	0.069647	-1103.130515	243.9	0

T3; trans-anti-anti, syn(H)	BP86/def-TZVP	-1103.200024	0.152870	-1103.047154	250.0	0.068900	-1103.131124	244.3	0
T3; trans-anti-anti, anti(H)	BP86/def-TZVP	-1103.200867	0.152814	-1103.048053	250.5	0.070132	-1103.130735	244.0	0
T3; trans-anti-anti, syn(H) (symmetrical)	BP86/def-TZVP	-1103.200881	0.152884	-1103.047997	248.5	0.069013	-1103.131868	242.7	0
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	-1103.199664	0.152923	-1103.046741	249.7	0.068230	-1103.131434	244.5	0
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	-1103.199154	0.152818	-1103.046336	249.5	0.068959	-1103.130195	243.7	0
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	-1103.200466	0.152666	-1103.04780	250.4	0.069360	-1103.131106	244.3	0
T4; trans-anti-syn	BP86/def-TZVP	-1103.209442	0.152172	-1103.057270	256.3	0.069649	-1103.139793	249.7	0
T4; trans-syn-anti	BP86/def-TZVP	-1103.212194	0.152239	-1103.059955	258.0	0.069886	-1103.142308	251.3	0
T4; trans-syn-anti	BP86/def2-TZVPP	-1103.262354	0.152148	-1103.110206	259.3	0.069891	-1103.192463	252.6	0
T4; trans-syn-syn	BP86/def-TZVP	-1103.211510	0.152215	-1103.059295	257.6	0.070007	-1103.141503	250.8	0
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	-1103.211691	0.152234	-1103.059457	255.7	0.069871	-1103.141820	248.9	0
T5; trans-anti-syn	BP86/def-TZVP	-1103.207395	0.152080	-1103.055315	255.1	0.069530	-1103.137865	248.5	0
T5; trans-syn-anti	BP86/def-TZVP	-1103.206349	0.152192	-1103.054157	254.4	0.068314	-1103.138035	248.6	0
T5; trans-syn-syn	BP86/def-TZVP	-1103.205257	0.152111	-1103.053146	253.7	0.068835	-1103.136422	247.6	0
T5; trans-anti-anti (symmetrical)	BP86/def-TZVP	-1103.209401	0.152131	-1103.05727	254.3	0.069643	-1103.139758	247.6	0
T6; anti-anti-syn	BP86/def-TZVP	-1103.189712	0.151375	-1103.038337	244.4	0.068950	-1103.120762	237.8	0
T6; anti-syn-anti	BP86/def-TZVP	-1103.190252	0.151366	-1103.038886	244.8	0.068512	-1103.121740	238.4	0
T6; anti-syn-syn	BP86/def-TZVP	-1103.190605	0.151374	-1103.039231	245.0	0.069214	-1103.121391	238.2	0
T6; anti-anti-anti (symmetrical)	BP86/def-TZVP	-1103.191634	0.151417	-1103.040217	243.6	0.068231	-1103.123403	237.4	0
10									
Anion									
Pyramidal	BP86/def-TZVP	-396.545269	0.046817	-396.498452		0.002491	-396.542778		0
	BP86/def2-TZVPP	-396.560182	0.046745	-396.513437		0.002409	-396.557773		0
	BP86/def2-TZVPPD	-396.562211	0.046729	-396.515482		0.002381	-396.559830		0
	B3LYP/def2-TZVPPD	-396.337980	0.047854	-396.290126		0.003954	-396.334026		0
	B3LYP/6-311+G(d,p)			-396.461507			-396.505256		0
	G4(MP2)			-395.913365			-395.957143		0
	W1RO			-396.503497			-396.547444		0
	CBS-APNO			-396.354140			-396.397710		0
Neutral									
T2	BP86/def-TZVP	-396.980622	0.057684	-396.922938	267.8	0.011796	-396.968826	261.1	0
	BP86/def2-TZVPP	-396.997238	0.057550	-396.939688	269.0	0.011550	-396.985688	262.2	0
	BP86/def2-TZVPPD	-396.998472	0.057531	-396.940941	268.5	0.011528	-396.986944	261.7	0
	B3LYP/def2-TZVPPD	-396.772719	0.059001	-396.713718	267.3	0.013657	-396.759062	260.4	0
	B3LYP/6-311+G(d,p)			-396.882396	265.6		-396.927541	258.7	0
	G4(MP2)			-396.334209	265.6		-396.379514	258.8	0
	W1RO			-396.924338	265.6		-396.969744	258.7	0
	CBS-APNO			-396.775450	265.9		-396.820224	258.9	0

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Anion									
	BP86/def-TZVP	-658.513570	0.081425	-658.432145		0.021771	-658.491798		0
	BP86/def2-TZVPP	-658.540177	0.081328	-658.458849		0.021683	-658.518494		0
	BP86/def2-TZVPPD	-658.542757	0.081235	-658.461522		0.020935	-658.521822		0
	B3LYP/def2-TZVPPD	-658.157888	0.083339	-658.074549		0.024135	-658.133753		0
	B3LYP/6-311+G(d,p)			-658.356677			-658.415158		0
	G4(MP2)			-657.449462			-657.508125		0
	CBS-APNO			-658.186709			-658.244858		0
T2; protonated on CN-1	BP86/def-TZVP	-658.940838	0.092376	-658.848462	262.7	0.031236	-658.909602	255.9	0
T2; protonated on CN-2	BP86/def-TZVP	-658.941348	0.092348	-658.849000	263.1	0.031355	-658.909993	256.1	0
T2; protonated on CN-3	BP86/def-TZVP	-658.941347	0.092350	-658.848997	263.1	0.031310	-658.910037	256.2	0
	BP86/def2-TZVPP	-658.969658	0.092197	-658.877461	264.2	0.030977	-658.938681	257.4	0
	BP86/def2-TZVPPD	-658.971598	0.092124	-658.879474	263.7	0.029584	-658.942014	257.4	0
	B3LYP/def2-TZVPPD	-658.585050	0.094574	-658.490476	262.5	0.033781	-658.551269	255.7	0
	B3LYP/6-311+G(d,p)			-658.769801	260.7		-658.829731	253.9	0
	G4(MP2)			-657.862713	260.8		-657.923005	254.1	0
	CBS-APNO			-658.599433	260.5		-658.658830	253.5	0
T4	BP86/def-TZVP	-658.908394	0.091647	-658.816747	242.8	0.029403	-658.878991	236.7	0
T5	BP86/def-TZVP	-658.919180	0.091892	-658.827288	249.4	0.030224	-658.888956	242.9	0
T6	BP86/def-TZVP	-658.922111	0.091737	-658.830374	251.4	0.029857	-658.892254	245.0	0

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Part of the name in () indicates that this group weakly exhibits this conformation.

Anion									
anti-syn; asymmetric	BP86/def-TZVP	-920.479451	0.116046	-920.363405		0.041524	-920.437927		0
	BP86/def2-TZVPP	-920.517651	0.115928	-920.401723		0.041507	-920.476144		0
	BP86/def2-TZVPPD	-920.520919	0.114788	-920.406131		0.043038	-920.477881		1
	B3LYP/def2-TZVPPD	-919.975370	0.117884	-919.857486		0.047633	-919.927737		1
	B3LYP/6-311+G(d,p)			-920.249602			-920.322557		0
	G4(MP2)			-918.985830			-919.059162		0
syn-syn; symmetric	BP86/def-TZVP	-920.480079	0.116042	-920.364037		0.041996	-920.438082		0
anti-anti; symmetric	BP86/def-TZVP	-920.477709	0.116039	-920.361670		0.040930	-920.436779		0
Neutral									
T2; protonated on CN-1; anti-syn	BP86/def-TZVP	-920.900635	0.126969	-920.773666	234.9	0.051317	-920.849318	251.9	0
	BP86/def2-TZVPP	-920.940491	0.126797	-920.813694	260.0	0.051106	-920.889385	253.0	0

	BP86/def2-TZVPPD	-920.943225	0.125669	-920.817556	259.7	0.052820	-920.890405	252.6	1
	B3LYP/def2-TZVPPD	-920.395797	0.129116	-920.266681	258.3	0.057846	-920.337951	251.1	1
	B3LYP/6-311+G(d,p)			-920.655992	256.5		-920.729905	249.3	0
	G4(MP2)			-919.392932	256.9		-919.467218	249.8	0
T2; protonated on CN-1; syn-syn	BP86/def-TZVP	-920.899040	0.105182	-920.793859	271.2	0.051588	-920.847452	250.6	0
T2; protonated on CN-1; rather anti-syn	BP86/def-TZVP	-920.898872	0.105224	-920.793649	271.5	0.051486	-920.847386	250.7	0
T2; protonated on CN-2; syn-syn	BP86/def-TZVP	-920.899030	0.105162	-920.793868	271.2	0.051531	-920.847499	250.6	0
T2; protonated on CN-2; anti-syn	BP86/def-TZVP	-920.900642	0.105228	-920.795414	272.6	0.051384	-920.849258	251.8	0
T2; protonated on CN-2; syn-anti	BP86/def-TZVP	-920.898869	0.105221	-920.793648	271.5	0.051485	-920.847384	250.7	0
T2; protonated on CN-2; anti-anti	BP86/def-TZVP	-920.898867	0.105212	-920.793655	272.6	0.051367	-920.847500	251.5	0
T4; cis-anti	BP86/def-TZVP	-920.868716	0.126334	-920.742382	239.3	0.049523	-920.819194	233.0	0
T4; cis-syn	BP86/def-TZVP	-920.870921	0.126332	-920.744589	240.3	0.050104	-920.820817	233.9	0
T4; trans-anti	BP86/def-TZVP	-920.867521	0.126327	-920.741194	239.6	0.049105	-920.818416	233.2	0
T4; trans-syn	BP86/def-TZVP	-920.871338	0.126363	-920.744975	240.9	0.050045	-920.821293	234.3	0
T5; cis-anti	BP86/def-TZVP	-920.879248	0.126479	-920.752769	245.8	0.050980	-920.828268	238.7	0
T5; cis-anti	BP86/def-TZVP	-920.879250	0.126483	-920.752767	245.8	0.051020	-920.828230	238.6	0
T5; cis-syn	BP86/def-TZVP	-920.882403	0.126559	-920.755844	247.3	0.051861	-920.830542	240.1	0
T5; trans-syn	BP86/def-TZVP	-920.879261	0.126487	-920.752774	245.8	0.050956	-920.828305	238.7	0
T5; trans-anti	BP86/def-TZVP	-920.882410	0.126563	-920.755847	248.8	0.051841	-920.830569	240.8	0
T6; anti-syn	BP86/def-TZVP	-920.878374	0.126397	-920.751977	245.3	0.050228	-920.828146	238.6	0
T6; syn-syn	BP86/def-TZVP	-920.884890	0.126515	-920.758375	248.9	0.051292	-920.833598	241.9	0
T6; anti-anti	BP86/def-TZVP	-920.881512	0.126457	-920.755055	248.3	0.051020	-920.830492	240.8	0
T6; syn-anti	BP86/def-TZVP	-920.881525	0.126455	-920.755070	247.3	0.048885	-920.832640	241.4	0
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Anion									
anti-syn-anti	BP86/def-TZVP	-1182.441154	0.150607	-1182.290547		0.062313	-1182.378841		0
anti-syn-syn	BP86/def-TZVP	-1182.439360	0.150622	-1182.288738		0.061437	-1182.377923		0
syn-syn-syn	BP86/def-TZVP	-1182.438355	0.150622	-1182.287733		0.062441	-1182.375914		0
anti-anti-anti	BP86/def-TZVP	-1182.441940	0.150625	-1182.291315		0.061703	-1182.380236		0
	BP86/def2-TZVPP	-1182.491515	0.150464	-1182.341051		0.061578	-1182.429937		0
	BP86/def2-TZVPPD	-1182.495503	0.146694	-1182.348809		0.064213	-1182.431290		3
	B3LYP/def2-TZVPPD	-1181.789127	0.152000	-1181.637127		0.069697	-1181.719430		2
	B3LYP/6-311+G(d,p)			-1182.138973			-1182.225550		0
	G4(MP2)			-1180.522159			-1180.60907		0
Neutral									
T2, anti-anti-syn	BP86/def-TZVP	-1182.856183	0.161547	-1182.694636	255.0	0.072174	-1182.784009	248.0	0
T2, anti-anti-anti	BP86/def-TZVP	-1182.858143	0.161563	-1182.696580	255.8	0.071907	-1182.786235	248.5	0
	BP86/def2-TZVPP	-1182.909556	0.161371	-1182.748185	257.0	0.071652	-1182.837904	249.7	0

	BP86/def2-TZVPPD	-1182.913153	0.157753	-1182.755400	256.6	0.074609	-1182.838544	249.3	3
	B3LYP/def2-TZVPPD	-1182.204831	0.163367	-1182.041464	255.2	0.079639	-1182.125192	248.3	2
	B3LYP/6-311+G(d,p)			-1182.540316	253.3		-1182.627589	246.0	0
	G4(MP2)			-1180.925138	254.4		-1181.012757	247.0	0
T2, anti-syn-syn	BP86/def-TZVP	-1182.853481	0.133972	-1182.719509	271.8	0.071292	-1182.782189	247.4	0
T2, syn-syn-syn	BP86/def-TZVP	-1182.851293	0.133979	-1182.717314	271.0	0.070890	-1182.780403	247.5	0
T4, trans-syn-anti	BP86/def-TZVP	-1182.828096	0.161027	-1182.667069	238.9	0.071031	-1182.757065	231.6	0
T4; cis-syn-anti	BP86/def-TZVP	-1182.826657	0.160997	-1182.665660	238.0	0.070428	-1182.756229	231.1	0
T4; trans-syn-syn	BP86/def-TZVP	-1182.825689	0.160988	-1182.664701	237.4	0.069339	-1182.756350	231.2	0
T4; cis-syn-syn (symmetrical)	BP86/def-TZVP	-1182.824790	0.161013	-1182.663777	237.4	0.071216	-1182.753574	230.7	0
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	-1182.827499	0.160992	-1182.666507	236.9	0.070393	-1182.757106	230.2	0
T4; cis-anti-anti	BP86/def-TZVP	-1182.827008	0.160928	-1182.666080	237.1	0.070756	-1182.756252	230.5	0
T4; trans-anti-syn	BP86/def-TZVP	-1182.824841	0.160906	-1182.663935	235.8	0.070358	-1182.754483	229.4	0
T4; cis-anti-syn	BP86/def-TZVP	-1182.823087	0.160909	-1182.662178	235.8	0.069331	-1182.753756	229.6	0
T5; trans-(anti)-anti	BP86/def-TZVP	-1182.839418	0.161154	-1182.678264	244.8	0.072996	-1182.766422	236.9	0
T5; cis-syn-anti	BP86/def-TZVP	-1182.829673	0.160997	-1182.668676	238.3	0.072226	-1182.757447	230.4	0
T5; trans-(anti)-syn	BP86/def-TZVP	-1182.836788	0.161077	-1182.675711	244.9	0.072117	-1182.764671	237.7	0
T5; cis-syn-(syn)	BP86/def-TZVP	-1182.828933	0.161002	-1182.667931	239.4	0.072043	-1182.756890	231.5	0
T5; trans-anti-anti	BP86/def-TZVP	-1182.838821	0.161164	-1182.677657	244.4	0.072667	-1182.766154	236.8	0
T5; cis-anti-anti	BP86/def-TZVP	-1182.830267	0.160984	-1182.669283	240.3	0.071737	-1182.758530	232.6	0
T5; trans-anti-syn	BP86/def-TZVP	-1182.835720	0.161049	-1182.674671	242.5	0.071688	-1182.764032	235.4	0
T5; cis-anti-(anti)	BP86/def-TZVP	-1182.830196	0.161009	-1182.669187	240.2	0.072142	-1182.758054	232.3	0
T6; trans-syn-anti	BP86/def-TZVP	-1182.837019	0.161070	-1182.675949	243.3	0.071753	-1182.765266	236.2	0
T6; cis-(anti)-anti	BP86/def-TZVP	-1182.838672	0.161136	-1182.677536	245.5	0.072262	-1182.766410	237.5	0
T6; trans-syn-(syn)	BP86/def-TZVP	-1182.836061	0.161039	-1182.675022	243.9	0.071390	-1182.764671	236.4	0
T6; cis-syn-syn (symmetrical)	BP86/def-TZVP	-1182.835070	0.161092	-1182.673978	243.9	0.071627	-1182.763443	236.9	0
T6; trans-anti-anti (symmetrical)	BP86/def-TZVP	-1182.835177	0.161021	-1182.674156	241.7	0.069689	-1182.765488	235.5	0
T6; cis-anti-anti	BP86/def-TZVP	-1182.840422	0.161110	-1182.679312	245.4	0.072262	-1182.768160	238.0	0
T6; trans-anti-(anti)	BP86/def-TZVP	-1182.834598	0.160997	-1182.673601	241.4	0.069680	-1182.764918	235.1	0
T6; cis-ani-syn	BP86/def-TZVP	-1182.835817	0.161050	-1182.674767	243.7	0.070796	-1182.765021	236.6	0
14									
Anion									
conformer I	BP86/def-TZVP	-1444.394467	0.185116	-1444.209351		0.085235	-1444.309232		0
conformer II	BP86/def-TZVP	-1444.394606	0.185057	-1444.209549		0.084463	-1444.310143		0
	BP86/def2-TZVPP	-1444.455659	0.184848	-1444.270811		0.084199	-1444.371460		0
conformer III; most stable from CosmoConf	BP86/def-TZVP	-1444.398421	0.185087	-1444.213334		0.085113	-1444.313308		0
	BP86/def2-TZVPP	-1444.459443	0.184893	-1444.274550		0.084896	-1444.374547		0
	BP86/def2-TZVPPD	-1444.464317	0.172971	-1444.291346		0.082882	-1444.381435		8

	B3LYP/6-311+G(d,p)			-1444.022448			-1444.119902		0
conformer IV	BP86/def-TZVP	-1444.398374	0.185060	-1444.213314		0.085023	-1444.313351		0
Neutral									
T4; conformer I	BP86/def-TZVP	-1444.773503	0.195401	-1444.578102	232.9	0.092612	-1444.680890	226.9	0
T4; conformer I	BP86/def-TZVP	-1444.777754	0.195439	-1444.582315	235.5	0.093606	-1444.684148	229.0	0
T4; conformer I	BP86/def-TZVP	-1444.777739	0.195433	-1444.582306	235.5	0.093544	-1444.684195	229.0	0
T4; conformer I	BP86/def-TZVP	-1444.777746	0.195435	-1444.582311	235.5	0.093557	-1444.684189	229.0	0
T4; conformer I	BP86/def-TZVP	-1444.777751	0.195439	-1444.582312	235.5	0.093626	-1444.684125	229.0	0
T4; conformer II	BP86/def-TZVP	-1444.776399	0.195410	-1444.580989	234.6	0.092180	-1444.684219	228.5	0
T4; conformer II	BP86/def-TZVP	-1444.776462	0.195377	-1444.581085	234.6	0.092043	-1444.684419	228.6	0
T4; conformer II	BP86/def-TZVP	-1444.778075	0.195435	-1444.582640	235.6	0.093099	-1444.684976	228.9	0
T4; conformer II	BP86/def-TZVP	-1444.774364	0.195388	-1444.578976	233.3	0.092250	-1444.682114	227.1	0
T4; conformer III	BP86/def-TZVP	-1444.780037	0.195406	-1444.584631	234.5	0.092816	-1444.687221	228.4	0
T4; conformer III	BP86/def-TZVP	-1444.780061	0.195416	-1444.584645	234.5	0.092839	-1444.687222	228.4	0
T4; conformer III	BP86/def-TZVP	-1444.780031	0.195411	-1444.584620	234.5	0.092746	-1444.687285	228.4	0
T4; conformer III	BP86/def-TZVP	-1444.780061	0.195425	-1444.584636	234.5	0.092879	-1444.687182	228.3	0
T4; conformer IV	BP86/def-TZVP	-1444.780005	0.195393	-1444.584612	234.5	0.092752	-1444.687253	228.3	0
T4; conformer IV	BP86/def-TZVP	-1444.780019	0.195394	-1444.584625	234.5	0.092813	-1444.687206	228.3	0
T4; conformer IV	BP86/def-TZVP	-1444.780011	0.195390	-1444.584621	234.5	0.092676	-1444.687335	228.4	0
T4; conformer IV	BP86/def-TZVP	-1444.780030	0.195399	-1444.584631	234.5	0.092932	-1444.687098	228.3	0
T5; conformer I	BP86/def-TZVP	-1444.782104	0.195512	-1444.586592	238.2	0.094211	-1444.687893	231.3	0
T5; conformer I	BP86/def-TZVP	-1444.781788	0.195468	-1444.586320	238.0	0.093430	-1444.688358	231.6	0
T5; conformer I	BP86/def-TZVP	-1444.782106	0.195512	-1444.586594	238.2	0.094322	-1444.687784	231.3	0
T5; conformer I	BP86/def-TZVP	-1444.782121	0.195520	-1444.586601	238.2	0.094326	-1444.687795	231.3	0
T5; conformer II	BP86/def-TZVP	-1444.779463	0.195391	-1444.584072	236.5	0.093368	-1444.686095	229.6	0
T5; conformer II	BP86/def-TZVP	-1444.777941	0.195409	-1444.582532	235.5	0.092541	-1444.685400	229.2	0
T5; conformer II	BP86/def-TZVP	-1444.776606	0.195335	-1444.581271	234.7	0.092698	-1444.683908	228.3	0
T5; conformer II	BP86/def-TZVP	-1444.777906	0.195387	-1444.582519	235.5	0.093810	-1444.684096	228.4	0
T5; conformer III	BP86/def-TZVP	-1444.782043	0.195481	-1444.586562	235.7	0.093777	-1444.688266	229.0	0
T5; conformer III	BP86/def-TZVP	-1444.782010	0.195459	-1444.586551	235.7	0.093662	-1444.688348	229.1	0
T5; conformer III	BP86/def-TZVP	-1444.782029	0.195452	-1444.586577	235.7	0.093640	-1444.688389	229.1	0
T5; conformer III	BP86/def-TZVP	-1444.782012	0.195470	-1444.586542	235.7	0.093732	-1444.688280	229.0	0
T5; conformer IV	BP86/def-TZVP	-1444.782005	0.195466	-1444.586539	235.7	0.093711	-1444.688294	229.0	0
T5; conformer IV	BP86/def-TZVP	-1444.781999	0.195457	-1444.586542	235.7	0.093727	-1444.688272	229.0	0
T5; conformer IV	BP86/def-TZVP	-1444.782009	0.195445	-1444.586564	235.7	0.093702	-1444.688307	229.0	0
T5; conformer IV	BP86/def-TZVP	-1444.782003	0.195454	-1444.586549	235.7	0.093619	-1444.688384	229.1	0
T6; conformer I	BP86/def-TZVP	-1444.784589	0.195525	-1444.589064	239.8	0.093804	-1444.690785	233.1	0
T6; conformer I	BP86/def-TZVP	-1444.784442	0.195508	-1444.588934	239.7	0.093707	-1444.690735	233.1	0
T6; conformer I	BP86/def-TZVP	-1444.784664	0.195528	-1444.589136	239.8	0.093856	-1444.690808	233.2	0

T6; conformer I	BP86/def-TZVP	-1444.784659	0.195524	-1444.589135	239.8	0.093813	-1444.690846	233.2	0
T6; conformer II	BP86/def-TZVP	-1444.786009	0.195494	-1444.590515	240.5	0.093413	-1444.692596	233.7	0
T6; conformer II	BP86/def-TZVP	-1444.787859	0.195532	-1444.592327	241.7	0.093479	-1444.694380	234.8	0
T6; conformer II	BP86/def2-TZVPP	-1444.851112	0.195292	-1444.655820	243.1	0.093143	-1444.757969	236.3	0
T6; conformer II	BP86/def-TZVP	-1444.785172	0.195502	-1444.589670	240.0	0.093229	-1444.691943	233.3	0
T6; conformer II	BP86/def-TZVP	-1444.782258	0.195434	-1444.586824	238.2	0.092437	-1444.689821	232.0	0
T6; conformer III	BP86/def-TZVP	-1444.788364	0.195505	-1444.592859	239.6	0.093675	-1444.694689	233.0	0
T6; conformer III	BP86/def-TZVP	-1444.788330	0.195495	-1444.592835	239.6	0.093627	-1444.694703	233.1	0
T6; conformer III	BP86/def-TZVP	-1444.788342	0.195504	-1444.592838	239.6	0.093634	-1444.694708	233.1	0
T6; conformer III	BP86/def2-TZVPP	-1444.851336	0.195272	-1444.656064	240.9	0.093222	-1444.758114	234.4	0
T6; conformer III	BP86/def2-TZVPPD	-1444.855872	0.181074	-1444.674798	242.1	0.094179	-1444.761693	232.3	10
T6; conformer III	B3LYP/6-311+G(d,p)			-1444.396548	236.2		-1444.495392	229.3	0
T6; conformer III	BP86/def-TZVP	-1444.788306	0.195499	-1444.592807	239.6	0.093513	-1444.694793	233.1	0
T6; conformer IV	BP86/def-TZVP	-1444.788302	0.195472	-1444.592830	239.6	0.093564	-1444.694738	233.0	0
T6; conformer IV	BP86/def-TZVP	-1444.788326	0.195490	-1444.592836	239.6	0.093656	-1444.694670	233.0	0
T6; conformer IV	BP86/def-TZVP	-1444.788334	0.195487	-1444.592847	239.6	0.093615	-1444.694719	233.0	0
T6; conformer IV	BP86/def-TZVP	-1444.788288	0.195485	-1444.592803	239.6	0.093496	-1444.694792	233.1	0
15									
Anion									
	BP86/def-TZVP	-92.891539	0.007963	-92.883576		-0.0143861	-92.905925		0
	B3LYP/def2-TZVPPD	-92.894504	0.007962	-92.886542		-0.014426	-92.908930		0
	B3LYP/6-311+G(d,p)			-92.880338			-92.902682		0
Neutral									
C-N-H	BP86/def-TZVP	-93.439333	0.018078	-93.421255	338.87468	0.0009865	-93.438347	327.8	0
H-C-N	BP86/def-TZVP	-93.463095	0.017952	-93.445143	353.86422	0.0022777	-93.460817	341.9	0
	B3LYP/def2-TZVPPD	-93.466651	0.020417	-93.446234	352.68775	0.005538	-93.461113	340.2	0
	B3LYP/6-311+G(d,p)			-93.434649	349.31115		-93.457492	341.9	0
16									
Anion									
	BP86/def-TZVP	-354.899269	0.041981	-354.857288		0.001916	-354.897353		0
	B3LYP/def2-TZVPPD	-354.914437	0.041953	-354.872484		0.001571	-354.912866		0
	B3LYP/6-311+G(d,p)			-354.811547			-354.851410		0
Neutal									
T1; $C(CN)_2$=CH(CN)	BP86/def-TZVP	-355.437345	0.054687	-355.382658	331.15071	0.014283	-355.423061	323.6	0
	B3LYP/def2-TZVPPD	-355.452729	0.054632	-355.398097	331.30291	0.013783	-355.438946	323.8	0
	B3LYP/6-311+G(d,p)			-355.336145	330.66624		-355.376488	323.2	0
T4; $C(CN\text{-}H)_2$=C(CN)	BP86/def-TZVP	-355.353640	0.052143	-355.301497	280.22258	0.010405	-355.343235	273.5	0

T6; $C(CN)_2$=C(CN-H)	BP86/def-TZVP	-355.393389	0.053931	-355.339458	304.04308	0.012341	-355.381049	297.2	0
T5; C(CN-H)$_2$=C(CN)	BP86/def-TZVP	-355.348482	0.052442	-355.296040	276.79807	0.009942	-355.338540	270.6	0
17									
Dianion									
$[B_{12}(CN)_{12}]^{2-}$	BP86/def-TZVP	-1413.480680	0.188055	-1413.292625		0.091658	-1413.389022		3
	BP86/def-TZVP	-1413.480695	0.188084	-1413.292611		0.091703	-1413.388992		3
	B3LYP/def2-TZVPPD	-1413.536355	0.186733	-1413.349622		0.089620	-1413.446735		3
	B3LYP/6-311+G(d,p)			-1413.152635			-1413.248443		
Anion									
$[B_{12}(CN)_{12}]^-$, protonated on CN	BP86/def-TZVP	-1413.964512	0.203011	-1413.761501	295.7	0.100872	-1413.863640	291.5	0
	B3LYP/def2-TZVPPD	-1414.021731	0.198238	-1413.823493	298.8	0.099193	-1413.922538	292.3	3
	B3LYP/6-311+G(d,p)			-1413.620604	295.1		-1413.718562	288.7	0
18									
Neutral									
$B_{12}(CN)_{12}H_2$, H-s dide by side	BP86/def-TZVP	-1414.350481	0.212976	-1414.137505	237.4	0.108904	-1414.241577	230.9	0
$B_{12}(CN)_{12}H_2$, 1 B between two H-s	BP86/def-TZVP	-1414.362171	0.210972	-1414.151199	246.0	0.109079	-1414.253092	238.1	2
	BP86/def-TZVP	-1414.362171	0.210013	-1414.152158			-1414.362171		3
$B_{12}(CN)_{12}H_2$, 2 B-s between two H-s	BP86/def-TZVP	-1414.365218	0.213296	-1414.151922	246.5	0.109359	-1414.255859	239.8	0
	B3LYP/def2-TZVPPD	-1414.423871	0.210204	-1414.213667	246.3	0.106791	-1414.317080	241.3	2
	B3LYP/6-311+G(d,p)			-1414.006915	243.9		-1414.106517	237.2	
19									
Anion									
$[CB_{11}(CN)_{12}]^-$	BP86/def-TZVP	-1426.559923	0.192538	-1426.367385		0.093785	-1426.466138		0
	B3LYP/def2-TZVPPD	-1426.616784	0.191696	-1426.425088		0.090700	-1426.526084		0
	B3LYP/6-311+G(d,p)			-1426.217878			-1426.314578		0
Neutral									
$CB_{11}(CN)_{12}H$, H on CN that is on C	BP86/def-TZVP	-1426.917444	0.202578	-1426.714866	219.5	0.101714	-1426.815730	213.1	0
$CB_{11}(CN)_{12}H$, H on CN that is on 1st row B	BP86/def-TZVP	-1426.930505	0.203348	-1426.727157	227.2	0.103048	-1426.827457	220.5	0
$CB_{11}(CN)_{12}H$, H on CN that is on 2nd row B	BP86/def-TZVP	-1426.938914	0.203342	-1426.735572	232.5	0.102888	-1426.836026	225.8	0
$CB_{11}(CN)_{12}H$, H on CN that is on opposite C	BP86/def-TZVP	-1426.941727	0.203149	-1426.738578	234.4	0.102169	-1426.839558	228.0	0
	B3LYP/def2-TZVPPD	-1427.000134	0.202346	-1426.797788	235.4	0.098932	-1426.901202	229.1	0
	B3LYP/6-311+G(d,p)			-1426.584522	231.6		-1426.683007	224.9	0

Table S10. DataDOI data repository filenames of title compounds in referred folders. See http://dx.doi.org/10.23673/re-436.

Compound	Basis set	GEO file	FR file	Folder	Cosmo file in CN_Cosmo folder
1					
Anion					
	BP86/def-TZVP	job_GEO_238	job_SP_239	CN_2	
	BP86/def2-TZVPP	job_GEO_491	job_SP_497	CN_1	COSMO-BP-TZVPD-FINE_17
	BP86/def2-TZVPPD	job_GEO_715	job_SP_717	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_719	job_SP_723	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1000		CN_GAU	
	G4(MP2)	JOB_1000_1		CN_GAU	
	W1RO	JOB_1000_2		CN_GAU	
	CBS-APNO	JOB_1000_3		CN_GAU	
Neutral					
T1	BP86/def-TZVP	job_GEO_242	job_SP_243	CN_2	
T2	BP86/def-TZVP	job_GEO_361	job_SP_362	CN_2	
	BP86/def2-TZVPP	job_GEO_492	job_SP_498	CN_1	COSMO-BP-TZVPD-FINE_19
	BP86/def2-TZVPPD	job_GEO_716	job_SP_718	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_720	job_SP_724	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1001		CN_GAU	
	G4(MP2)	JOB_1001_1		CN_GAU	
	W1RO	JOB_1001_2		CN_GAU	
	CBS-APNO	JOB_1001_3		CN_GAU	
2					
Anion					
	BP86/def-TZVP	job_GEO_223	job_SP_231	CN_2	
	BP86/def2-TZVPP	job_GEO_501	job_SP_503	CN_1	COSMO-BP-TZVPD-FINE_21
	BP86/def2-TZVPPD	job_GEO_725	job_SP_729	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_727	job_SP_731	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1002		CN_GAU	
	G4(MP2)	JOB_1002_1		CN_GAU	
	W1RO	JOB_1002_2		CN_GAU	
	CBS-APNO	JOB_1002_3		CN_GAU	
Neutral					
T1	BP86/def-TZVP	job_GEO_224	job_SP_232	CN_2	
	BP86/def2-TZVPP	job_GEO_502	job_SP_505	CN_1	COSMO-BP-TZVPD-FINE_23
	BP86/def2-TZVPPD	job_GEO_726	job_SP_730	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_728	job_SP_732	CN_1	

	B3LYP/6-311+G(d,p)	JOB_1003		CN_GAU	
	G4(MP2)	JOB_1003_1		CN_GAU	
	W1RO	JOB_1003_2		CN_GAU	
	CBS-APNO	JOB_1003_3		CN_GAU	
T3; eclipsed(H)	BP86/def-TZVP	job_GEO_225	job_SP_233	CN_2	
T3; syn(H)	BP86/def-TZVP	job_GEO_78	job_SP_80	CN_1	
T3; anti(H)	BP86/def-TZVP	job_GEO_82	job_SP_83	CN_1	
T4	BP86/def-TZVP	job_GEO_32	job_SP_34	CN_1	COSMO-BP-TZVPD-FINE_316
T5	BP86/def-TZVP	job_GEO_226	job_SP_234	CN_2	COSMO-BP-TZVPD-FINE_314
T6	BP86/def-TZVP	job_GEO_33	job_SP_35	CN_1	
3					
Anion					
	BP86/def-TZVP	job_GEO_363	job_SP_364	CN_2	
	BP86/def2-TZVPP	job_GEO_506	job_SP_508	CN_1	COSMO-BP-TZVPD-FINE_26
	BP86/def2-TZVPPD	job_GEO_733	job_SP_760	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_734	job_SP_761	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1004		CN_GAU	
	G4(MP2)	JOB_1004_1		CN_GAU	
	W1RO	JOB_1004_2		CN_GAU	
	CBS-APNO	JOB_1004_3		CN_GAU	
Neutral					
T1	BP86/def-TZVP	job_GEO_247	job_SP_250	CN_2	
T2	BP86/def-TZVP	job_GEO_248	job_SP_251	CN_2	
	BP86/def2-TZVPP	job_GEO_507	job_SP_509	CN_1	COSMO-BP-TZVPD-FINE_28
	BP86/def2-TZVPPD	job_GEO_735	job_SP_762	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_736	job_SP_763	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1005		CN_GAU	
	G4(MP2)	JOB_1005_1		CN_GAU	
	W1RO	JOB_1005_2		CN_GAU	
	CBS-APNO	JOB_1005_3		CN_GAU	
4					
Anion					
anti	BP86/def-TZVP	job_GEO_254	job_SP_263	CN_2	
	BP86/def2-TZVPP	job_GEO_510	job_SP_515	CN_1	COSMO-BP-TZVPD-FINE_116
	BP86/def2-TZVPPD	job_GEO_737	job_SP_776	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_738	job_SP_777	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1006		CN_GAU	

	G4(MP2)	JOB_1006_1		CN_GAU	
	W1RO	JOB_1006_2		CN_GAU	
	CBS-APNO	JOB_1006_3		CN_GAU	
syn	BP86/def-TZVP	job_GEO_332	job_SP_340	CN_2	
	BP86/def2-TZVPP	job_GEO_511	job_SP_516	CN_1	COSMO-BP-TZVPD-FINE_30
Neutral					
T1; syn	BP86/def-TZVP	job_GEO_255	job_SP_264	CN_2	
T1; anti	BP86/def-TZVP	job_GEO_333	job_SP_341	CN_2	
T2; anti	BP86/def-TZVP	job_GEO_258	job_SP_267	CN_2	
	BP86/def2-TZVPP	job_GEO_514	job_SP_518	CN_1	COSMO-BP-TZVPD-FINE_118
	BP86/def2-TZVPPD	job_GEO_739	job_SP_778	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_740	job_SP_779	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1007		CN_GAU	
	G4(MP2)	JOB_1007_1		CN_GAU	
	W1RO	JOB_1007_2		CN_GAU	
	CBS-APNO	JOB_1007_3		CN_GAU	
T2; syn	BP86/def-TZVP	job_GEO_335	job_SP_343	CN_2	
	BP86/def2-TZVPP	job_GEO_513	job_SP_517	CN_1	COSMO-BP-TZVPD-FINE_32
T3; trans, eclipsed(H)	BP86/def-TZVP	job_GEO_256	job_SP_265	CN_2	
T3; trans, syn(H)	BP86/def-TZVP	job_GEO_85	job_SP_95	CN_1	
T3; cis, anti(H)	BP86/def-TZVP	job_GEO_22	job_SP_23	CN_1	
T3; cis, syn(H)	BP86/def-TZVP	job_GEO_84	job_SP_94	CN_1	
T4; trans	BP86/def-TZVP	job_GEO_257	job_SP_266	CN_2	
T4; cis	BP86/def-TZVP	job_GEO_334	job_SP_342	CN_2	
T5; trans	BP86/def-TZVP	job_GEO_37	job_SP_45	CN_1	
T5; cis	BP86/def-TZVP	job_GEO_38	job_SP_42	CN_1	
T6; anti	BP86/def-TZVP	job_GEO_40	job_SP_44	CN_1	
T6; syn	BP86/def-TZVP	job_GEO_39	job_SP_43	CN_1	
5					
Anion					
Anion; anti-syn (syn facing forward)	BP86/def-TZVP	job_GEO_259	job_SP_269	CN_2	
Anion; anti-syn (syn facing backward)	BP86/def-TZVP	job_GEO_471	job_SP_475	CN_1	COSMO-BP-TZVPD-FINE_120
	BP86/def2-TZVPP	job_GEO_522	job_SP_524	CN_1	COSMO-BP-TZVPD-FINE_53
anti-anti	BP86/def-TZVP	job_GEO_19	job_SP_20	CN_1	COSMO-BP-TZVPD-FINE_122
	BP86/def2-TZVPP	job_GEO_741	job_SP_770	CN_1	
	BP86/def2-TZVPPD	job_GEO_742	job_SP_771	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_775	job_SP_794	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1008		CN_GAU	

	G4(MP2)	JOB_1008_1		CN_GAU	
	CBS-APNO	JOB_1008_3		CN_GAU	
syn-syn	BP86/def-TZVP	job_GEO_25	job_SP_26	CN_1	COSMO-BP-TZVPD-FINE_124
Neutral					
T1; anti-syn (syn facing forward)	BP86/def-TZVP	job_GEO_472	job_SP_476	CN_1	COSMO-BP-TZVPD-FINE_126
T1; anti-syn (syn facing backward)	BP86/def-TZVP	job_GEO_260	job_SP_270	CN_2	
	BP86/def2-TZVPP	job_GEO_523	job_SP_525	CN_1	COSMO-BP-TZVPD-FINE_55
T1; syn-syn	BP86/def-TZVP	job_GEO_27	job_SP_29	CN_1	COSMO-BP-TZVPD-FINE_128
T1; anti-anti	BP86/def-TZVP	job_GEO_795	job_SP_812	CN_1	COSMO-BP-TZVPD-FINE_130
	BP86/def2-TZVPP	job_GEO_744	job_SP_773	CN_1	
	BP86/def2-TZVPPD	job_GEO_745	job_SP_774	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_758	job_SP_772	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1009		CN_GAU	
	G4(MP2)	JOB_1009_1		CN_GAU	
	CBS-APNO	JOB_1009_3		CN_GAU	
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_261	job_SP_271	CN_2	
T3; cis-anti, syn(H)	BP86/def-TZVP	job_GEO_91	job_SP_104	CN_1	
T3; trans-anti, syn(H)	BP86/def-TZVP	job_GEO_338	job_SP_349	CN_2	
T3; trans-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_96	job_SP_105	CN_1	
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_75	job_SP_106	CN_1	
T3; cis-syn, syn(H)	BP86/def-TZVP	job_GEO_92	job_SP_107	CN_1	
T3; trans-syn, syn(H)	BP86/def-TZVP	job_GEO_67	job_SP_76	CN_1	
T3; trans-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_93	job_SP_108	CN_1	
T4; cis-anti	BP86/def-TZVP	job_GEO_262	job_SP_272	CN_2	
T4; trans-anti	BP86/def-TZVP	job_GEO_339	job_SP_347	CN_2	
T4; cis-syn	BP86/def-TZVP	job_GEO_51	job_SP_72	CN_1	
T4; trans-syn	BP86/def-TZVP	job_GEO_47	job_SP_59	CN_1	
T5; trans-anti	BP86/def-TZVP	job_GEO_48	job_SP_64	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_49	job_SP_65	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_50	job_SP_57	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_905	job_SP_906	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_60	job_SP_68	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_61	job_SP_73	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_62	job_SP_70	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_63	job_SP_74	CN_1	
6					
Anion					
	BP86/def-TZVP	job_GEO_273	job_SP_290	CN_2	

	BP86/def2-TZVPP	job_GEO_538	job_SP_540	CN_1	COSMO-BP-TZVPD-FINE_38
	BP86/def2-TZVPPD	job_GEO_747	job_SP_799	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_748	job_SP_800	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1010		CN_GAU	
	G4(MP2)	JOB_1010_1		CN_GAU	
	W1RO	JOB_1010_2		CN_GAU	
	CBS-APNO	JOB_1010_3		CN_GAU	
Neutral					
T1	BP86/def-TZVP	job_GEO_274	job_SP_291	CN_2	
T2	BP86/def-TZVP	job_GEO_275	job_SP_292	CN_2	
	BP86/def2-TZVPP	job_GEO_539	job_SP_542	CN_1	COSMO-BP-TZVPD-FINE_40
	BP86/def2-TZVPPD	job_GEO_749	job_SP_801	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_750	job_SP_802	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1011		CN_GAU	
	G4(MP2)	JOB_1011_1		CN_GAU	
	W1RO	JOB_1011_2		CN_GAU	
	CBS-APNO	JOB_1011_3		CN_GAU	
7					
Anion					
	BP86/def-TZVP	job_GEO_276	job_SP_293	CN_2	
	BP86/def2-TZVPP	job_GEO_544	job_SP_570	CN_1	COSMO-BP-TZVPD-FINE_57
	BP86/def2-TZVPPD	job_GEO_751	job_SP_803	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_752	job_SP_804	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1012		CN_GAU	
	G4(MP2)	JOB_1012_1		CN_GAU	
	W1RO	JOB_1012_2		CN_GAU	
	CBS-APNO	JOB_1012_3		CN_GAU	
Neutral					
T3 = T1; anti(H)	BP86/def-TZVP	job_GEO_277	job_SP_296	CN_2	
T3 = T1; syn(H)	BP86/def-TZVP	job_GEO_307	job_SP_309	CN_2	
T2 = T4	BP86/def-TZVP	job_GEO_278	job_SP_295	CN_2	
T2 = T5	BP86/def-TZVP	job_GEO_109	job_SP_113	CN_1	
	BP86/def2-TZVPP	job_GEO_543	job_SP_571	CN_1	COSMO-BP-TZVPD-FINE_71
	BP86/def2-TZVPPD	job_GEO_753	job_SP_805	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_754	job_SP_806	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1013		CN_GAU	
	G4(MP2)	JOB_1013_1		CN_GAU	
	W1RO	JOB_1013_2		CN_GAU	

	CBS-APNO	JOB_1013_3		CN_GAU	
T6	BP86/def-TZVP	job_GEO_110	job_SP_112	CN_1	
8					
Anion					
syn-syn	BP86/def-TZVP	job_GEO_279	job_SP_297	CN_2	COSMO-BP-TZVPD-FINE_132
anti-syn	BP86/def-TZVP	job_GEO_308	job_SP_316	CN_2	COSMO-BP-TZVPD-FINE_134
	BP86/def2-TZVPP	job_GEO_755	job_SP_807	CN_1	
	BP86/def2-TZVPPD	job_GEO_756	job_SP_808	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_757	job_SP_809	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1014		CN_GAU	
	G4(MP2)	JOB_1014_1		CN_GAU	
	CBS-APNO	JOB_1014_3		CN_GAU	
anti-anti	BP86/def-TZVP	job_GEO_116	job_SP_117	CN_1	
	BP86/def2-TZVPP	job_GEO_545	job_SP_572	CN_1	COSMO-BP-TZVPD-FINE_73
Neutral					
T1; syn-syn	BP86/def-TZVP	job_GEO_175	job_SP_184	CN_1	
T1; anti-anti	BP86/def-TZVP	job_GEO_114	job_SP_118	CN_1	
T1; anti-syn = syn-anti	BP86/def-TZVP	job_GEO_280	job_SP_298	CN_2	
T2; anti-anti	BP86/def-TZVP	job_GEO_283	job_SP_301	CN_2	
	BP86/def2-TZVPP	job_GEO_546	job_SP_573	CN_1	COSMO-BP-TZVPD-FINE_114
T2; syn-anti	BP86/def-TZVP	job_GEO_317	job_SP_322	CN_2	COSMO-BP-TZVPD-FINE_136
	BP86/def2-TZVPP	job_GEO_810	job_SP_811	CN_1	
	BP86/def2-TZVPPD	job_GEO_823	job_SP_826	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_824	job_SP_835	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1015		CN_GAU	
	G4(MP2)	JOB_1015_1		CN_GAU	
	CBS-APNO	JOB_1015_3		CN_GAU	
T2; syn-syn	BP86/def-TZVP	job_GEO_123	job_SP_124	CN_1	COSMO-BP-TZVPD-FINE_138
T3; cis-anti, anti(H)	BP86/def-TZVP	job_GEO_315	job_SP_321	CN_2	
T3; cis-anti, syn(H)	BP86/def-TZVP	job_GEO_152	job_SP_153	CN_1	
T3; cis-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_170	job_SP_171	CN_1	
T3; trans-anti, syn(H)	BP86/def-TZVP	job_GEO_154	job_SP_155	CN_1	
T3; trans-anti, anti(H)	BP86/def-TZVP	job_GEO_162	job_SP_174	CN_1	
T3; cis-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_157	job_SP_167	CN_1	
T3; trans-syn, syn(H)	BP86/def-TZVP	job_GEO_159	job_SP_168	CN_1	
T3; trans-syn, anti(H)	BP86/def-TZVP	job_GEO_161	job_SP_173	CN_1	
T4; cis-anti	BP86/def-TZVP	job_GEO_122	job_SP_125	CN_1	
T4; cis-syn	BP86/def-TZVP	job_GEO_121	job_SP_126	CN_1	

T4; trans-syn	BP86/def-TZVP	job_GEO_127	job_SP_128	CN_1	
T4; trans-anti	BP86/def-TZVP	job_GEO_289	job_SP_300	CN_2	
T5; trans-anti	BP86/def-TZVP	job_GEO_129	job_SP_133	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_130	job_SP_134	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_131	job_SP_135	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_132	job_SP_136	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_137	job_SP_142	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_150	job_SP_151	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_141	job_SP_147	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_140	job_SP_149	CN_1	
9					
Anion					
symmetrical	BP86/def-TZVP	job_GEO_285	job_SP_302	CN_2	
	BP86/def2-TZVPP	job_GEO_549	job_SP_574	CN_1	COSMO-BP-TZVPD-FINE_63
	BP86/def2-TZVPPD	job_GEO_837	job_SP_841	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_838	job_SP_845	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1016		CN_GAU	
	G4(MP2)	JOB_1016_1		CN_GAU	
asymmetrical	BP86/def-TZVP	job_GEO_327	job_SP_331	CN_2	
	BP86/def2-TZVPP	job_GEO_550	job_SP_575	CN_1	COSMO-BP-TZVPD-FINE_65
Neutral					
T1; asymmetrical, anti-syn-syn; H facing backward	BP86/def-TZVP	job_GEO_286	job_SP_303	CN_2	COSMO-BP-TZVPD-FINE_306
T1; symmetrical, syn-syn-syn; H facing backward	BP86/def-TZVP	job_GEO_324	job_SP_328	CN_2	COSMO-BP-TZVPD-FINE_308
T1; symmetrical, anti-anti-anti; H facing backward	BP86/def-TZVP	job_GEO_178	job_SP_182	CN_1	
	BP86/def2-TZVPP	job_GEO_547	job_SP_576	CN_1	
	BP86/def2-TZVPPD	job_GEO_869	job_SP_871	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_840	job_SP_846	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1017		CN_GAU	
	G4(MP2)	JOB_1017_1		CN_GAU	
T1; asymmetrical, anti-anti-syn; H facing backward	BP86/def-TZVP	job_GEO_177	job_SP_181	CN_1	COSMO-BP-TZVPD-FINE_310
T3; trans-syn-syn, eclipsed(H)	BP86/def-TZVP	job_GEO_287	job_SP_306	CN_2	
T3; trans-syn-syn, anti(H)	BP86/def-TZVP	job_GEO_325	job_SP_329	CN_2	
T3; trans-syn-syn, syn(H)	BP86/def-TZVP	job_GEO_209	job_SP_210	CN_1	
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	job_GEO_211	job_SP_233	CN_1	
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	job_GEO_212	job_SP_223	CN_1	
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_213	job_SP_225	CN_1	
T3; trans-anti-anti, syn(H)	BP86/def-TZVP	job_GEO_220	job_SP_226	CN_1	
T3; trans-anti-anti, anti(H)	BP86/def-TZVP	job_GEO_221	job_SP_234	CN_1	

T3; trans-anti-anti, syn(H) (symmetrical)	BP86/def-TZVP	job_GEO_216	job_SP_228	CN_1	
T3; trans-syn-anti, syn(H)	BP86/def-TZVP	job_GEO_217	job_SP_229	CN_1	
T3; trans-syn-anti, anti(H)	BP86/def-TZVP	job_GEO_218	job_SP_235	CN_1	
T3; trans-syn-anti, eclipsed(H)	BP86/def-TZVP	job_GEO_231	job_SP_232	CN_1	
T4; trans-anti-syn	BP86/def-TZVP	job_GEO_288	job_SP_304	CN_2	COSMO-BP-TZVPD-FINE_140
T4; trans-syn-anti	BP86/def-TZVP	job_GEO_179	job_SP_187	CN_1	
T4; trans-syn-anti	BP86/def2-TZVPP	job_GEO_548	job_SP_577	CN_1	COSMO-BP-TZVPD-FINE_69
T4; trans-syn-syn	BP86/def-TZVP	job_GEO_185	job_SP_189	CN_1	COSMO-BP-TZVPD-FINE_142
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_183	job_SP_186	CN_1	COSMO-BP-TZVPD-FINE_144
T5; trans-anti-syn	BP86/def-TZVP	job_GEO_193	job_SP_198	CN_1	
T5; trans-syn-anti	BP86/def-TZVP	job_GEO_190	job_SP_199	CN_1	
T5; trans-syn-syn	BP86/def-TZVP	job_GEO_192	job_SP_200	CN_1	
T5; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_191	job_SP_207	CN_1	
T6; anti-anti-syn	BP86/def-TZVP	job_GEO_197	job_SP_202	CN_1	
T6; anti-syn-anti	BP86/def-TZVP	job_GEO_194	job_SP_203	CN_1	
T6; anti-syn-syn	BP86/def-TZVP	job_GEO_196	job_SP_206	CN_1	
T6; anti-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_195	job_SP_208	CN_1	
10					
Anion					
Pyramidal	BP86/def-TZVP	job_GEO_365	job_SP_366	CN_2	
	BP86/def2-TZVPP	job_GEO_551	job_SP_578	CN_1	COSMO-BP-TZVPD-FINE_75
	BP86/def2-TZVPPD	job_GEO_847	job_SP_872	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_848	job_SP_873	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1018		CN_GAU	
	G4(MP2)	JOB_1018_1		CN_GAU	
	W1RO	JOB_1018_2		CN_GAU	
	CBS-APNO	JOB_1018_3		CN_GAU	
Neutral					
T2	BP86/def-TZVP	job_GEO_352	job_SP_355	CN_2	
	BP86/def2-TZVPP	job_GEO_552	job_SP_579	CN_1	COSMO-BP-TZVPD-FINE_77
	BP86/def2-TZVPPD	job_GEO_849	job_SP_874	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_850	job_SP_875	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1019		CN_GAU	
	G4(MP2)	JOB_1019_1		CN_GAU	
	W1RO	JOB_1019_2		CN_GAU	
	CBS-APNO	JOB_1019_3		CN_GAU	
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Anion					
	BP86/def-TZVP	job_GEO_356	jos_SP_390	CN_2	
	BP86/def2-TZVPP	job_GEO_553	job_SP_598	CN_1	COSMO-BP-TZVPD-FINE_79
	BP86/def2-TZVPPD	job_GEO_851	job_SP_878	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_852	job_SP_879	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1020		CN_GAU	
	G4(MP2)	JOB_1020_1		CN_GAU	
	W1RO	JOB_1020_2		CN_GAU	
	CBS-APNO	JOB_1020_3		CN_GAU	
T2; protonated on CN-1	BP86/def-TZVP	job_GEO_360	job_SP_392	CN_2	
T2; protonated on CN-2	BP86/def-TZVP	job_GEO_238	job_SP_242	CN_1	
T2; protonated on CN-3	BP86/def-TZVP	job_GEO_239	job_SP_243	CN_1	
	BP86/def2-TZVPP	job_GEO_554	job_SP_599	CN_1	COSMO-BP-TZVPD-FINE_81
	BP86/def2-TZVPPD	job_GEO_853	job_SP_880	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_854	job_SP_881	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1021		CN_GAU	
	G4(MP2)	JOB_1021_1		CN_GAU	
	W1RO	JOB_1021_2		CN_GAU	
	CBS-APNO	JOB_1021_3		CN_GAU	
T4	BP86/def-TZVP	job_GEO_244	job_SP_245	CN_1	
T5	BP86/def-TZVP	job_GEO_389	job_SP_391	CN_1	
T6	BP86/def-TZVP	job_GEO_237	job_SP_241	CN_1	
12					
Anion					
anti-syn; asymmetric	BP86/def-TZVP	job_GEO_454	job_SP_457	CN_2	
	BP86/def2-TZVPP	job_GEO_555	job_SP_600	CN_1	COSMO-BP-TZVPD-FINE_83
	BP86/def2-TZVPPD	job_GEO_855	job_SP_882	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_856	job_SP_883	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1022		CN_GAU	
	G4(MP2)	JOB_1022_1		CN_GAU	
	CBS-APNO	JOB_1022_3		CN_GAU	
syn-syn; symmetric	BP86/def-TZVP	job_GEO_455	job_SP_458	CN_2	COSMO-BP-TZVPD-FINE_147
anti-anti; symmetric	BP86/def-TZVP	job_GEO_456	job_SP_459	CN_2	COSMO-BP-TZVPD-FINE_149
Neutral					
T2; protonated on CN-1; anti-syn	BP86/def-TZVP	job_GEO_114	job_SP_115	CN_3	
	BP86/def2-TZVPP	job_GEO_556	job_SP_601	CN_1	COSMO-BP-TZVPD-FINE_85
	BP86/def2-TZVPPD	job_GEO_857	job_SP_884	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_858	job_SP_885	CN_1	

	B3LYP/6-311+G(d,p)	JOB_1023		CN_GAU	
	G4(MP2)	JOB_1023 _1		CN_GAU	
	CBS-APNO	JOB_1023_3		CN_GAU	
T2; protonated on CN-1; syn-syn	BP86/def-TZVP	job_GEO_253	job_SP_304	CN_1	COSMO-BP-TZVPD-FINE_151
T2; protonated on CN-1; rather anti-syn	BP86/def-TZVP	job_GEO_252	job_SP_305	CN_1	COSMO-BP-TZVPD-FINE_167
T2; protonated on CN-2; syn-syn	BP86/def-TZVP	job_GEO_255	job_SP_306	CN_1	
T2; protonated on CN-2; anti-syn	BP86/def-TZVP	job_GEO_250	job_SP_307	CN_1	
T2; protonated on CN-2; syn-anti	BP86/def-TZVP	job_GEO_251	job_SP_308	CN_1	
T2; protonated on CN-2; anti-anti	BP86/def-TZVP	job_GEO_254	job_SP_309	CN_1	COSMO-BP-TZVPD-FINE_169
T4; cis-anti	BP86/def-TZVP	job_GEO_113	job_SP_116	CN_3	
T4; cis-syn	BP86/def-TZVP	job_GEO_258	job_SP_267	CN_1	
T4; trans-anti	BP86/def-TZVP	job_GEO_256	job_SP_295	CN_1	
T4; trans-syn	BP86/def-TZVP	job_GEO_257	job_SP_296	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_261	job_SP_297	CN_1	
T5; cis-anti	BP86/def-TZVP	job_GEO_262	job_SP_283	CN_1	
T5; cis-syn	BP86/def-TZVP	job_GEO_286	job_SP_298	CN_1	
T5; trans-syn	BP86/def-TZVP	job_GEO_259	job_SP_299	CN_1	
T5; trans-anti	BP86/def-TZVP	job_GEO_260	job_SP_300	CN_1	
T6; anti-syn	BP86/def-TZVP	job_GEO_264	job_SP_301	CN_1	
T6; syn-syn	BP86/def-TZVP	job_GEO_266	job_SP_302	CN_1	
T6; anti-anti	BP86/def-TZVP	job_GEO_268	job_SP_281	CN_1	
T6; syn-anti	BP86/def-TZVP	job_GEO_265	job_SP_281	CN_1	
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Anion					
anti-syn-anti	BP86/def-TZVP	job_GEO_129	job_SP_136	CN_3	COSMO-BP-TZVPD-FINE_155
anti-syn-syn	BP86/def-TZVP	job_GEO_131	job_SP_138	CN_3	COSMO-BP-TZVPD-FINE_157
syn-syn-syn	BP86/def-TZVP	job_GEO_248	job_SP_249	CN_1	COSMO-BP-TZVPD-FINE_153
anti-anti-anti	BP86/def-TZVP	job_GEO_137	job_SP_139	CN_3	
	BP86/def2-TZVPP	job_GEO_557	job_SP_604	CN_1	COSMO-BP-TZVPD-FINE_87
	BP86/def2-TZVPPD	job_GEO_859	job_SP_886	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_860	job_SP_887	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1024		CN_GAU	
	G4(MP2)	JOB_1024 _1		CN_GAU	
Neutral					
T2, anti-anti-syn	BP86/def-TZVP	job_GEO_127	job_SP_134	CN_3	COSMO-BP-TZVPD-FINE_159
T2, anti-anti-anti	BP86/def-TZVP	job_GEO_100	job_SP_106	CN_3	COSMO-BP-TZVPD-FINE_161
	BP86/def2-TZVPP	job_GEO_558	job_SP_603	CN_1	COSMO-BP-TZVPD-FINE_89
	BP86/def2-TZVPPD	job_GEO_861	job_SP_888	CN_1	

	B3LYP/def2-TZVPPD	job_GEO_862	job_SP_889	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1025			
	G4(MP2)	JOB_1025 _1			
T2, anti-syn-syn	BP86/def-TZVP	job_GEO_313	job_SP_314	CN_1	COSMO-BP-TZVPD-FINE_163
T2, syn-syn-syn	BP86/def-TZVP	job_GEO_312	job_SP_315	CN_1	COSMO-BP-TZVPD-FINE_165
T4, trans-syn-anti	BP86/def-TZVP	job_GEO_128	job_SP_135	CN_3	
T4; cis-syn-anti	BP86/def-TZVP	job_GEO_317	job_SP_366	CN_1	
T4; trans-syn-syn	BP86/def-TZVP	job_GEO_318	job_SP_367	CN_1	
T4; cis-syn-syn (symmetrical)	BP86/def-TZVP	job_GEO_319	job_SP_373	CN_1	
T4; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_320	job_SP_374	CN_1	
T4; cis-anti-anti	BP86/def-TZVP	job_GEO_321	job_SP_375	CN_1	
T4; trans-anti-syn	BP86/def-TZVP	job_GEO_322	job_SP_371	CN_1	
T4; cis-anti-syn	BP86/def-TZVP	job_GEO_323	job_SP_372	CN_1	
T5; trans-(anti)-anti	BP86/def-TZVP	job_GEO_340	job_SP_377	CN_1	
T5; cis-syn-anti	BP86/def-TZVP	job_GEO_333	job_SP_378	CN_1	
T5; trans-(anti)-syn	BP86/def-TZVP	job_GEO_334	job_SP_383	CN_1	
T5; cis-syn-(syn)	BP86/def-TZVP	job_GEO_343	job_SP_380	CN_1	
T5; trans-anti-anti	BP86/def-TZVP	job_GEO_336	job_SP_381	CN_1	
T5; cis-anti-anti	BP86/def-TZVP	job_GEO_337	job_SP_382	CN_1	
T5; trans-anti-syn	BP86/def-TZVP	job_GEO_338	job_SP_392	CN_1	
T5; cis-anti-(anti)	BP86/def-TZVP	job_GEO_347	job_SP_385	CN_1	
T6; trans-syn-anti	BP86/def-TZVP	job_GEO_348	job_SP_402	CN_1	
T6; cis-(anti)-anti	BP86/def-TZVP	job_GEO_341	job_SP_394	CN_1	
T6; trans-syn-(syn)	BP86/def-TZVP	job_GEO_342	job_SP_403	CN_1	
T6; cis-syn-syn (symmetrical)	BP86/def-TZVP	job_GEO_335	job_SP_401	CN_1	
T6; trans-anti-anti (symmetrical)	BP86/def-TZVP	job_GEO_344	job_SP_404	CN_1	
T6; cis-anti-anti	BP86/def-TZVP	job_GEO_345	job_SP_398	CN_1	
T6; trans-anti-(anti)	BP86/def-TZVP	job_GEO_346	job_SP_405	CN_1	
T6; cis-ani-syn	BP86/def-TZVP	job_GEO_339	job_SP_400	CN_1	
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Anion					
conformer I	BP86/def-TZVP	job_GEO_86	job_SP_88	CN_3	COSMO-BP-TZVPD-FINE_175
conformer II	BP86/def-TZVP	job_GEO_406	job_SP_421	CN_1	
	BP86/def2-TZVPP	job_GEO_559	job_SP_595	CN_1	COSMO-BP-TZVPD-FINE_91
conformer III; most stable from CosmoConf	BP86/def-TZVP	job_GEO_675	job_SP_676	CN_1	COSMO-BP-TZVPD-FINE_171
	BP86/def2-TZVPP	job_GEO_863	job_SP_890	CN_1	
	BP86/def2-TZVPPD	job_GEO_864	job_SP_891	CN_1	
	B3LYP/6-311+G(d,p)	JOB_1026		CN_GAU	

	G4(MP2)	JOB_1026 _1		CN_GAU	
conformer IV	BP86/def-TZVP	job_GEO_677	job_SP_680	CN_1	COSMO-BP-TZVPD-FINE_173
Neutral					
T4; conformer I	BP86/def-TZVP	job_GEO_109	job_SP_117	CN_3	
T4; conformer I	BP86/def-TZVP	job_GEO_437	job_SP_449	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_440	job_SP_450	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_443	job_SP_451	CN_1	
T4; conformer I	BP86/def-TZVP	job_GEO_446	job_SP_452	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_410	job_SP_424	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_422	job_SP_433	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_416	job_SP_429	CN_1	
T4; conformer II	BP86/def-TZVP	job_GEO_419	job_SP_434	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_1)	job_SP_685	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_2)	job_SP_686	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_3)	job_SP_687	CN_1	
T4; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T4_4)	job_SP_688	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_1)	job_SP_698	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_2)	job_SP_699	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_3)	job_SP_700	CN_1	
T4; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T4_4)	job_SP_701	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_448	job_SP_453	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_465	job_SP_466	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_442	job_SP_461	CN_1	
T5; conformer I	BP86/def-TZVP	job_GEO_447	job_SP_456	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_409	job_SP_423	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_414	job_SP_427	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_415	job_SP_430	CN_1	
T5; conformer II	BP86/def-TZVP	job_GEO_418	job_SP_432	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_1)	job_SP_689	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_2)	job_SP_690	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_3)	job_SP_691	CN_1	
T5; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T5_4)	job_SP_692	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_1)	job_SP_702	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_2)	job_SP_703	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_3)	job_SP_704	CN_1	
T5; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T5_4)	job_SP_705	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_438	job_SP_457	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_441	job_SP_462	CN_1	
T6; conformer I	BP86/def-TZVP	job_GEO_444	job_SP_463	CN_1	COSMO-BP-TZVPD-FINE_178

T6; conformer I	BP86/def-TZVP	job_GEO_445	job_SP_464	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_411	job_SP_425	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_412	job_SP_426	CN_1	
T6; conformer II	BP86/def2-TZVPP	job_GEO_560	job_SP_602	CN_1	COSMO-BP-TZVPD-FINE_93
T6; conformer II	BP86/def-TZVP	job_GEO_417	job_SP_431	CN_1	
T6; conformer II	BP86/def-TZVP	job_GEO_420	job_SP_435	CN_1	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_1)	job_SP_693	CN_1	COSMO-BP-TZVPD-FINE_180
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_2)	job_SP_694	CN_1	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_3)	job_SP_695	CN_1	
T6; conformer III	BP86/def2-TZVPP	job_GEO_866	job_SP_892	CN_1	
T6; conformer III	BP86/def2-TZVPPD	job_GEO_867	job_SP_893	CN_1	
T6; conformer III	B3LYP/6-311+G(d,p)	JOB_1027		CN_GAU	
T6; conformer III	G4(MP2)	JOB_1027 _1		CN_GAU	
T6; conformer III	BP86/def-TZVP	CN_684 (14_AN_1_T6_4)	job_SP_696	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_1)	job_SP_706	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_2)	job_SP_707	CN_1	
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_3)	job_SP_708	CN_1	COSMO-BP-TZVPD-FINE_182
T6; conformer IV	BP86/def-TZVP	CN_697 (14_AN_2_T6_4)	job_SP_709	CN_1	
15					
Anion					
	BP86/def-TZVP	job_GEO_539	job_SP_545	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_561	job_SP_605	CN_1	COSMO-BP-TZVPD-FINE_95
	B3LYP/6-311+G(d,p)	JOB_1029		CN_GAU	
Neutral					
C-N-H	BP86/def-TZVP	job_GEO_540	job_SP_546	CN_3	
H-C-N	BP86/def-TZVP	job_GEO_541	job_SP_547	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_562	job_SP_606	CN_1	COSMO-BP-TZVPD-FINE_97
	B3LYP/6-311+G(d,p)	JOB_1030		CN_GAU	
16					
Anion					
	BP86/def-TZVP	job_GEO_542	job_SP_548	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_563	job_SP_607	CN_1	COSMO-BP-TZVPD-FINE_99
	B3LYP/6-311+G(d,p)	JOB_1031		CN_GAU	
Neutal					
T1; C(CN)2=CH(CN)	BP86/def-TZVP	job_GEO_552	job_SP_553	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_564	job_SP_608	CN_1	COSMO-BP-TZVPD-FINE_101
	B3LYP/6-311+G(d,p)	JOB_1032		CN_GAU	

T4; C(CN-H)2=C(CN)	BP86/def-TZVP	job_GEO_544	job_SP_550	CN_3	
T6; C(CN)2=C(CN-H)	BP86/def-TZVP	job_GEO_477	job_SP_483	CN_1	
T5; C(CN-H)2=C(CN)	BP86/def-TZVP	job_GEO_478	job_SP_484	CN_1	
17					
Dianion					
[B12(CN)12]2-	BP86/def-TZVP	job_GEO_364	job_SP_369	CN_3	
	BP86/def-TZVP	job_GEO_486	job_SP_487	CN_1	
	B3LYP/def2-TZVPPD	job_GEO_565	job_SP_594	CN_1	COSMO-BP-TZVPD-FINE_103
	B3LYP/6-311+G(d,p)	JOB_1033		CN_GAU	
Anion					
[B12(CN)12]-, protonated on CN	BP86/def-TZVP	job_GEO_365	job_SP_370	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_566	job_SP_597	CN_1	COSMO-BP-TZVPD-FINE_105
	B3LYP/6-311+G(d,p)	JOB_1034		CN_GAU	
18					
Neutral					
B12(CN)12H2, H-s dide by side	BP86/def-TZVP	job_GEO_373	job_SP_379	CN_3	
B12(CN)12H2, 1 B between two H-s	BP86/def-TZVP	job_GEO_376	job_SP_380	CN_3	
	BP86/def-TZVP	job_GEO_488	job_SP_537	CN_1	
B12(CN)12H2, 2 B-s between two H-s	BP86/def-TZVP	job_GEO_372	job_SP_381	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_567	job_SP_593	CN_1	COSMO-BP-TZVPD-FINE_107
	B3LYP/6-311+G(d,p)	JOB_1035		CN_GAU	
19					
Anion					
[CB11(CN)12]-	BP86/def-TZVP	job_GEO_391	job_SP_396	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_568	job_SP_592	CN_1	COSMO-BP-TZVPD-FINE_109
	B3LYP/6-311+G(d,p)	JOB_1036		CN_GAU	
Neutral					
CB11(CN)12-H, H on CN that is on C	BP86/def-TZVP	job_GEO_392	job_SP_397	CN_3	
CB11(CN)12-H, H on CN that is on 1st row B	BP86/def-TZVP	job_GEO_393	job_SP_398	CN_3	
CB11(CN)12-H, H on CN that is on 2nd row B	BP86/def-TZVP	job_GEO_394	job_SP_399	CN_3	
CB11(CN)12-H, H on CN that is on opposite C	BP86/def-TZVP	job_GEO_395	job_SP_400	CN_3	
	B3LYP/def2-TZVPPD	job_GEO_569	job_SP_596	CN_1	COSMO-BP-TZVPD-FINE_111
	B3LYP/6-311+G(d,p)	JOB_1037		CN_GAU	

Table S11. DataDOI data repository filenames of auxiliary acids in the COSMO-RS folder. See http://dx.doi.org/10.23673/re-436.

Compd name	CAS		FILENAME		
			ANION		NEUTRAL
NH_2-TCNP	98555-43-2		COSMO-BP-TZVPD-FINE_184	T4	COSMO-BP-TZVPD-FINE_186
				T5	COSMO-BP-TZVPD-FINE_188
				T3	COSMO-BP-TZVPD-FINE_190
Me-TCNP	24943-63-3		COSMO-BP-TZVPD-FINE_192	T4	COSMO-BP-TZVPD-FINE_194
				T5	COSMO-BP-TZVPD-FINE_196
3,4-$(MeO)_2$-C_6H_3-TCNP	1261286-75-2	Conf 1	COSMO-BP-TZVPD-FINE_198	T4	COSMO-BP-TZVPD-FINE_289
				T5	COSMO-BP-TZVPD-FINE_202
		Conf 2		T4	COSMO-BP-TZVPD-FINE_204
				T5	COSMO-BP-TZVPD-FINE_304
4-MeO-C_6H_4-TCNP	1261286-76-3		COSMO-BP-TZVPD-FINE_208	T4	COSMO-BP-TZVPD-FINE_210
				T5	COSMO-BP-TZVPD-FINE_212
Ph-TCNP	96463-47-7		COSMO-BP-TZVPD-FINE_214	T4	COSMO-BP-TZVPD-FINE_216
				T5	COSMO-BP-TZVPD-FINE_219
3-CF_3-C_6H_4-TCNP	2226486-85-5	Conf 1	COSMO-BP-TZVPD-FINE_223	T4	COSMO-BP-TZVPD-FINE_225
				T5	COSMO-BP-TZVPD-FINE_227
		Conf 2		T4	COSMO-BP-TZVPD-FINE_229
				T5	COSMO-BP-TZVPD-FINE_233
H-TCNP	32019-26-4		COSMO-BP-TZVPD-FINE_235	T3	COSMO-BP-TZVPD-FINE_237
				T4	COSMO-BP-TZVPD-FINE_239
Br-TCNP	100125-09-5		COSMO-BP-TZVPD-FINE_243	T4	COSMO-BP-TZVPD-FINE_245
				T5	COSMO-BP-TZVPD-FINE_247
3,5-$(CF_3)_2$-C_6H_3-TCNP	1261286-79-6		COSMO-BP-TZVPD-FINE_249	T4	COSMO-BP-TZVPD-FINE_251
				T5	COSMO-BP-TZVPD-FINE_253
Cl-TCNP	1261286-80-9		COSMO-BP-TZVPD-FINE_256	T4	COSMO-BP-TZVPD-FINE_258
				T5	COSMO-BP-TZVPD-FINE_260
CN-CH_2-TCNP	2638-14-4		COSMO-BP-TZVPD-FINE_274	T4	COSMO-BP-TZVPD-FINE_276
				T5	COSMO-BP-TZVPD-FINE_278
CF_3-TCNP	1261286-81-0		COSMO-BP-TZVPD-FINE_221	T4	COSMO-BP-TZVPD-FINE_264
			COSMO-BP-TZVPD-FINE_262	T5	COSMO-BP-TZVPD-FINE_266