Supporting Information

Computational modelling of ammonia addition on partially reduced graphene oxide flakes

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1. Computational methods – for finite-sized molecules

To verify the chosen functional and basis set pair, a series of calculations were carried out, in which the size of the basis set was gradually increased (Table S1) and in which the applied functional was varied (Table S2). We concentrated on the transition state energies of Figure 8 while looking at the effect of the different computational parameters since activation barriers determine most of the reaction's conditions.

Increasing the basis set with additional diffuse and/or polarisation functions had no notable effect on the activation energies (cc. 1 kcal/mol, see Table S1). Applying a basis set around the same level as 6-31+g but from a different family (cc-p-VDZ) resulted in minor changes in the coronene system's transition states and a slight increase in **$TS_{0\text{-}1}$** for ovalene (4 kcal/mol difference). Based on these results, we concluded that the 6-31+g basis set is sufficiently large to be applied for the targeted systems.

Table S1: The effect of increased basis set size
Calculated relative energies (ΔE) of the rate-determining transition state steps for the coronene and ovalene based reactions (see Figure 8), using an increasing level of basis functions for the optimisation and the Dunning type cc-pVDZ basis set.

Methods	**Relative energies of coronene model, ΔE [kcal/mol]**		**Relative energies of ovalene model, ΔE [kcal/mol]**	
	CO-$TS_{0\text{-}1}$	**CO-$TS_{1\text{-}2}$**	**$TS_{0\text{-}1}$**	**$TS_{1\text{-}2}$**
B3LYP/6-31+G*	31.4	30.4	33.8	34.0
B3LYP/6-31+G(2d,p)	30.1	31.4	33.7	34.8
B3LYP /6-311+G(2d,p)	30.7	32.0	34.3	35.4
B3LYP /6-311++G(2d,p)	30.7	32.0	34.3	35.4
B3LYP /cc-pVDZ	33.7	29.8	37.8	33.8

To compare the performance of the B3LYP functional, we calculated the transition state energies with other functionals, such as B97D, which was successfully applied for similarly large condensed systems before.[ref] We can see, based on the results in Table S2, that the B97D functional consistently gives smaller energy barriers with 6 kcal/mol for epoxy migration and 8 kcal/mol for the ammonia addition. This significant decrease in energies presumably results from some form of dispersion correction built into the B97D functional. Upon including Grimme's D2 dispersion correction formula in the B3LYP calculations, we found a similar decrease level in the ammonia addition barrier (less than 6 kcal/mol) but only

a negligible difference in the $TS_{0\text{-}1}$ barriers. Furthermore, by applying the hybrid functional of wB97XD, which is supposedly more sophisticated than B97D, we calculated transition state energies much closer but slightly higher than the original B3LYP results. Further investigations by calculating single point energies of the epoxy migration on a coronene system were carried out with the MP2 method and predicted even higher energies than DFT functionals. Overall, we concluded that B3LYP without dispersion correction gives similar results to other, higher-level functionals (wB97XD) and, therefore, is sufficient for describing possible reactions between ammonia and oxidised PAH systems.

Table S2: Test calculations with B3LYP, B97D, B3LYP-D2, wB97XD functionals and the MP2 method

Calculated relative energies (ΔE) of the rate-determining transition state steps for the coronene and ovalene based reactions (see Figure 8), using different type of functionals and methods. In cases where two different methods were applied, we used the following notations: A//B where A is the method used for the geometry optimisation, and B is for single point energy. These single point energies results are also shown underlined and italic in the table. [a]This value is related to a structurally different transition state optimised with the wB97XD method.

Methods	**Relative energies of coronene model, ΔE [kcal/mol]**		**Relative energies of ovalene model, ΔE [kcal/mol]**	
	COR-$TS_{0\text{-}1}$	**COR-$TS_{1\text{-}2}$**	**$TS_{0\text{-}1}$**	**$TS_{1\text{-}2}$**
b3lyp/6-31+g*	31.4	30.4	33.8	34.0
b3lyp/6-31+g*// b3lyp/6-31+g* EmpiricalDispersion= GD2	*31.9*	*24.3*	*31.8*	*28.3*
b97d/6-31+g*	24.6	22.6	27.1	25.7
b97/6-31+g*// b98/6-31+g*	*30.9*	*29.5*	*35.2*	*33.6*
b97d/6-31+g(2d,p)	24.8	23.6	27.2	26.6
wb97xd/6-31+g(2d,p)	34.4	26.5[a]	39.9	34.2
wb97xd/6-31+g(2d,p)// wb97xd/6-311++g(2d,p)	*34.9*			
wb97xd/6-31+g(2d,p)// mp2/6-31+g(2d,p)	*41.3*			
wb97xd/6-31+g(2d,p)// mp2/6-311++g(2d,p)	*41.9*			

Table S3: Test calculations with the IEFPCM solvent method

Single point energies calculated for each b3lyp/6-31+g* geometry optimised steps of the relevant reaction mechanisms (Figure 8, 11, 13) using the integral equation formulation variant of the polarisable continuum solvent model (IEFPCM) implemented in Gaussian09 to represent a homogenous aqueous media.

Notation	ΔE [kcal/mol] without IEFPCM method	ΔE [kcal/mol] with IEFPCM method
0	0.0	0.0
TS_{0-1}	33.8	29.6
1	10.6	10.8
TS_{1-2}	34.0	32.9
2	-8.4	-7.5
Notation	**ΔE [kcal/mol] without IEFPCM method**	**ΔE [kcal/mol] with IEFPCM method**
0-H_2O	0.0	0.0
TS_{0-1}-H_2O	29.2	26.0
1-H_2O	10.0	9.9
TS_{1-2}-H_2O	29.8	28.9
2-H_2O	6.6	1.3
TS_{2-3}-H_2O	8.5	4.1
3-H_2O	-9.7	-10.0
Notation	**ΔE [kcal/mol] without IEFPCM method**	**ΔE [kcal/mol] with IEFPCM method**
0-2NH_3	0.0	0.0
TS_{0-1}-2NH_3	33.3	28.8
1-2NH_3	11.2	10.8
TS_{1-2}-2NH_3	31.1	30.0
2-2NH_3	-6.3	-9.6

2. Computational methods – periodic DFT

Periodic DFT calculations were performed to justify the applied finite-sized models. The original 32 carbon unit cell with epoxy groups was taken from Ref 40. In this referenced material, we optimised the cell parameters using the irreducible unit cell of pristine graphene on the PBE/(C): 6-21G*, (O): 8-411 theoretical level. Then the optimised cell parameters were fixed, and a supercell with 32 carbon atoms was created, keeping only the translational symmetry of the unit cell. The following parameters are constants in our PBC models: a,b=9.88 Å, α,β=90° and γ=120°.

Basis sets were tested for small systems (epoxy-benzene, benzene, oxirane, ethene), and the chosen basis set pair proved to be in good agreement with 6-31G or aug-cc-pvtz both in relative energies and geometrical parameters. We note that further increase of the basis set size and the addition of diffuse functions might have caused the artificial overlapping of basis functions within the neighbouring until cell. Therefore, we accepted the already established basis functions of the Crystal09 software developers' and did not attempt to modify the basis set used for molecular calculations. We also tested the effect using the hybrid functional PBE, but we found that applying PBE0 is more relevant to electronic properties, such as band gaps, than in the case of geometrical optimisations.

We tested the density of the k mesh on the 32C unit cell with four-epoxy groups. (An original k mesh convergence was done for the pristine graphene too). We compared the parameters shown in Table S4 and found that the bandgap and the chosen bond lengths are unchanged from shrinking factor 4. The energy difference becomes acceptably small at 8x8; therefore, we applied this shrinking factor for the geometry optimisations.

Table S4: k mesh convergence for the four-epoxy group containing 32C unit cell
Energy differences between the different shrinking factor values are presented in a.u., the bandgap in eV and the most important bond lengths in Å

Shrinking factor	**2**	**4**	**6**	**8**	**10**
E diff (a.u.)	-	-1.22E-03	-1.74E-05	-6.47E-07	-3.50E-08
Band gap (eV)	0.942	0.932	0.932	0.932	0.932
C – C (Å	1.490	1.491	1.491	1.491	1.491
C = C (Å)	1.433	1.433	1.433	1.433	1.433
C – O (Å)	1.465	1.465	1.465	1.465	1.465

3. Applied models

Periodic DFT calculations were carried out to search for stable epoxy group formations with different epoxy-group densities. Formation energy was used to evaluate the energetic stability of the systems, which is the energy of the reduced graphene oxides (E_f) compared to the electronic energy of the n epoxy group-containing unit cell (E_{RGO}), to the energy of the same sized clean graphene cell (E_G) and n number of oxygen atoms ($E_{O_2}/2$) optimised in vacuum.

$$E_f = E_{RGO} - (E_G + nE_{O_2}/2) \qquad \text{Eq. 1.}$$

Besides the formation energy of whole epoxy group conformations, the relative energy gain or loss due to an additional epoxy group in an already existing formation can carry useful information too. Relative energies derived to a single epoxy group (E_f/O) are calculated by comparing the energy of n epoxy group-containing system to the energy of the most stable $n-1$ structure:

$$E_f/O = E_{RGO,n} - (E_{RGO,(n-1)} + E_{O_2}/2) \qquad \text{Eq.2}$$

We gradually increased the number of epoxy groups on the surface, described by the so-called epoxy group density: the oxygen-carbon ratio (O/C%) within the applied 32 carbon atom containing unit cell. We considered both sides of the graphene sheet when we probed for the most stable group formation with different epoxy group densities. The full account of considered formations is summarised in Table S5.

By comparing the calculated formation energies of the most stable structures in all epoxy group densities (Figure S1), we found that they only vary within a small energy range (19-25 kcal/mol). All E_f energies are positive, suggesting that the formation of epoxy groups leads to the disturbance of the aromatic framework. However, plotting the formation energy per oxygen atom (E_f/O) in Figure S1 shows that after breaking the delocalised electron net with one epoxy group, the addition of further epoxy groups does not require significant energy investment. On the contrary, in the case of bigger than two epoxy ensembles adding one more epoxy group and increasing the coverage is getting more energetically favourable (with 0.0 – 4.5 kcal/mol).

Table S5: **Summary of periodic DFT calculations with different O/C% cells**

Calculated formation energies (E_f) for the investigated epoxy group configurations for each epoxy group density using the PBE functional. Formation energies are evaluated for the whole structure and an additional epoxy group by comparing the system to the most stable structure with one less epoxy group (E_f/O).

O/C (%)	epoxy groups	absolute E a.u.	E_f (kcal/mol)	E_f/O (kcal/mol)
0.0	graphene	-1217.555731		
3.1	*1*	*-1292.619640*	*19.2*	-
6.3	2a	-1367.672824	45.2	25.9
6.3	2b	-1367.696542	30.3	11.1
6.3	2c	-1367.700915	27.5	8.3
6.3	2d	-1367.696209	30.5	11.3
6.3	2e	-1367.669787	47.1	27.9
6.3	2f	-1367.707139	23.6	4.4
6.3	*2g*	*-1367.707526*	*23.4*	*4.2*
9.4	3a	-1442.785780	33.6	10.2
9.4	*3b*	*-1442.802041*	*23.4*	*0.0*
9.4	3c	-1442.801355	23.8	0.4
9.4	3d	-1442.781650	36.2	12.8
9.4	3e	-1442.795917	27.2	3.9
9.4	3f	-1442.767856	44.9	21.5
9.4	3g	-1442.777549	38.8	15.4
12.5	4a	-1517.867978	41.4	17.9
12.5	4b	-1517.887914	28.8	5.4
12.5	4c	-1517.885975	30.1	6.7
12.5	4d	-1517.887662	29.0	5.6
12.5	*4e*	*-1517.896988*	*23.1*	*-0.3*
15.6	5a	-1592.941557	54.5	31.4
15.6	5b	-1592.960294	42.7	19.6
15.6	*5c*	*-1592.989396*	*24.5*	*1.3*
15.6	5d	-1592.983098	28.4	5.3
15.6	5e	-1592.964488	40.1	17.0
15.6	5f	-1592.962721	41.2	18.1
15.6	5g	-1592.971426	35.8	12.6
15.6	5h	-1592.978169	31.5	8.4
15.6	5i	-1592.953145	47.2	24.1
15.6	5j	-1592.948895	49.9	26.8
15.6	5k	-1592.981737	29.3	6.1
15.6	5l	-1592.973868	34.2	11.1
18.8	6a	-1668.005196	73.9	49.4
18.8	*6b*	*-1668.091153*	*20.0*	*-4.5*
18.8	6c	-1668.082857	25.2	0.7
18.8	6d	-1668.087862	22.0	-2.5
18.8	6e	-1668.068405	34.2	9.7

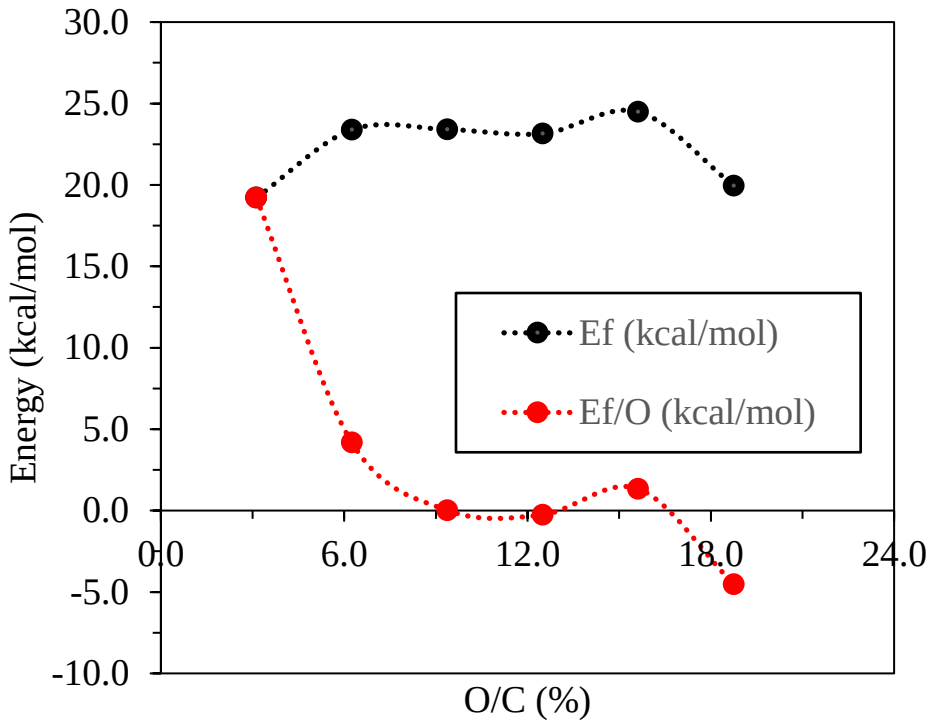


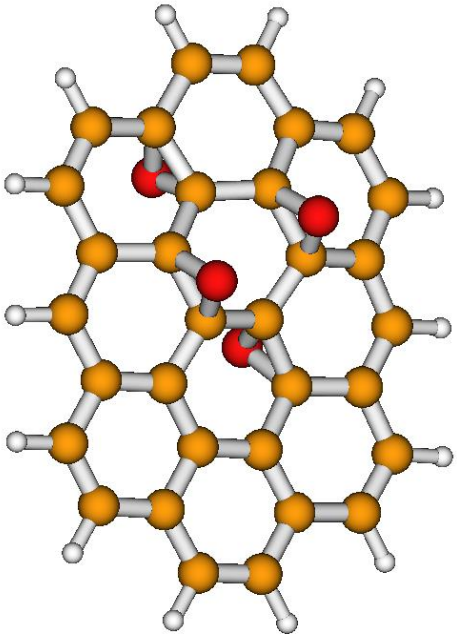
Figure S1: Calculated formation (full black circles, E_f) energies together with their relative derivates for a single epoxy group (full red circles E_f/O) plotted for each studied epoxy group density (O/C %) in kcal/mol.

Previous studies suggest that certain epoxy group formations are more stable on the graphene-oxide surface than others. One particularly stable conformation is found for four epoxy groups in which two epoxy groups are facing "up" on the opposite sides of the same carbon ring, while two epoxy group is facing "down" on the other side of the plane, parallel to each other. Only two different arrangements of this four-epoxy group formation are possible relative to the ovalene if we exclude the ones in which the epoxy groups are directly on the edges. Calculating the formation energies of these systems by using the following equation:

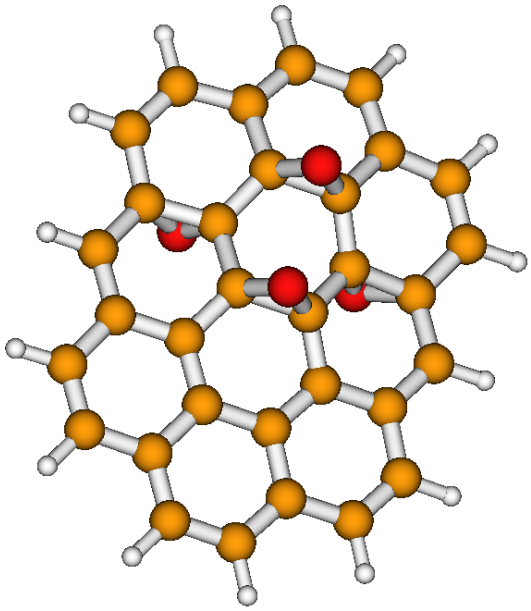
$$E_{formation}=E_{ovalene\_4epoxy}-(E_{ovalene}+2O_2) \qquad \text{Eq. 3.}$$

predicts structure 1 in Figure S2 thermodynamically stable with -22.1 kcal/mol, while formation 2 is practically unstable with 0.3 kcal/mol. Therefore, we only used formation 1 to study the ammonia adsorption.

Figure S2: formation 1 (left) and formation 2 (right) are the two possible four-epoxy group arrangements on ovalene, represented by balls and sticks images. Their relative energies are written in (kcal/mol). (red=O, orange=C, white=H)

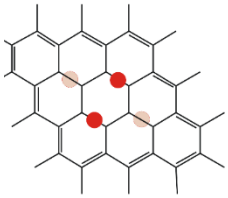
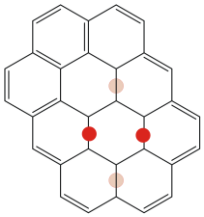
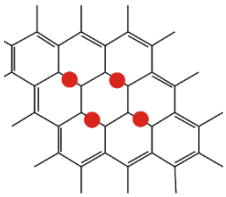
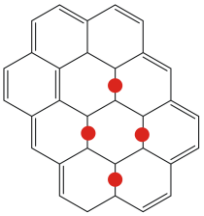
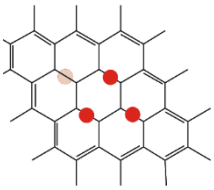
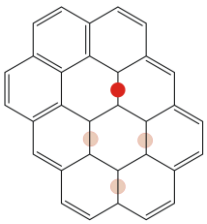
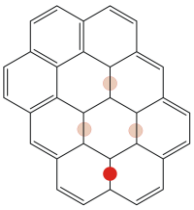
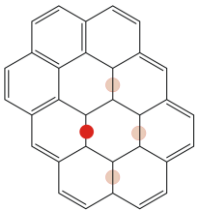


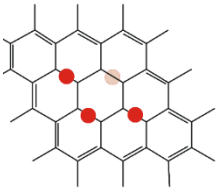
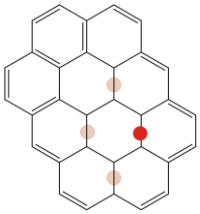
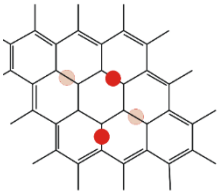
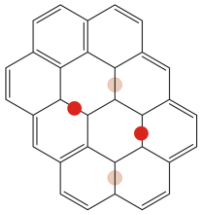
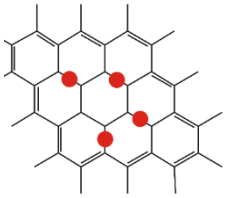
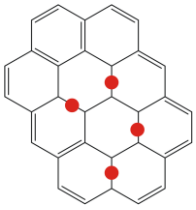
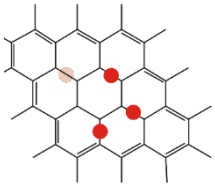
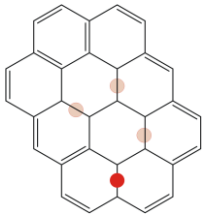
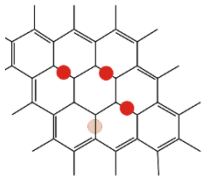
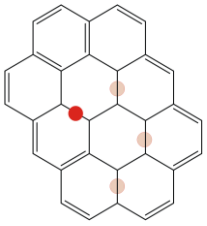
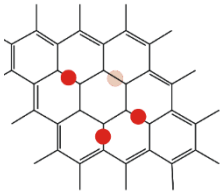
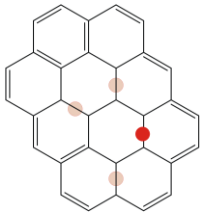
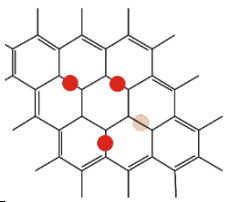
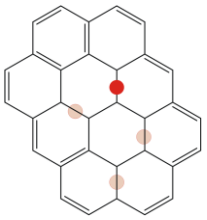
-22.1 kcal/mol



0.3 kcal/mol

Table S6: Comparison of the relative stabilities of periodic and ovalene based models. Relative energies of different four-epoxy group formations compared to the reference structures containing two up- and two down-facing epoxy groups and calculated with periodic DFT (ΔE_{PBC}) or with the ovalene molecule (ΔE_{OV}).

32 C unit cell + 4 epoxy	**ΔE_{PBC} (kcal/mol)**	**OV + 4 epoxy**	**ΔE_{OV} (kcal/mol)**
	0.00		0.00
	18.17		4.24
	6.48		1.91
			2.70
	9.07		1.11

			0.44
	9.09		10.87
	30.03		18.05
	16.42		16.15
	21.39		18.65
	18.39		15.37
	18.61		15.15

4. Ammonia addition on the used PRGO models

Figure S3: Electrostatic potential energy maps of the COR and OV molecules

The Isodensity surface value was set to 0.01 a.u. The potential energy scale is between -0.0772 a.u. (red) and +0.0772 a.u. (blue).

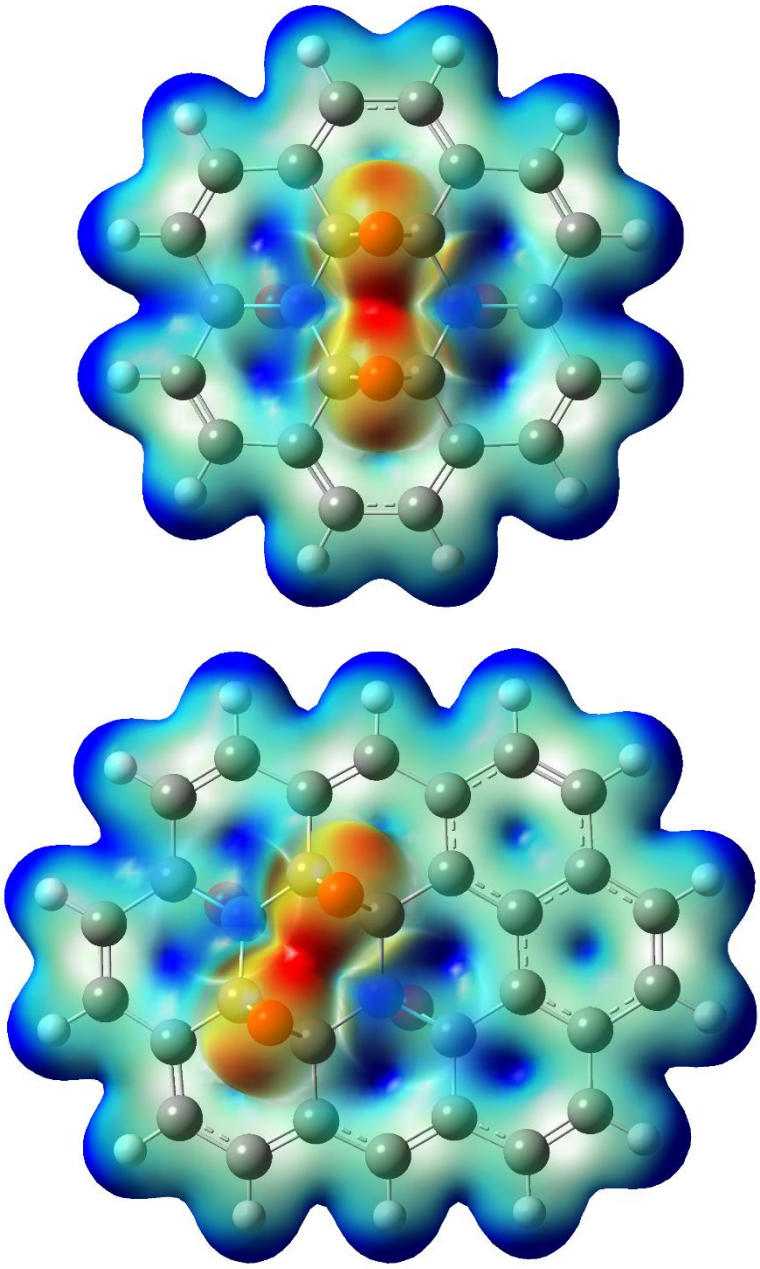


Table S7: Atomic distances and natural charges for the coronene model in Figure 8

Optimised atomic distances (Å) and calculated natural atomic charges (a.u.) at each step of the ammonia addition mechanism on a coronene based PRGO model in Figure 8.

Atomic distances (Å)						
	N-C1	**N-H1**	**O1-H1**	**O1-C1**	**O1-C2**	**O1-C3**
COR-0	4.227	1.020	2.307	1.439	1.438	2.464
COR-TS$_{0\text{-}1}$	4.541	1.022	2.108	2.188	1.389	2.275

COR-1	3.786	1.020	2.376	2.486	1.438	1.468
COR-TS$_{1-2}$	2.070	1.033	1.794	2.483	1.390	1.974
COR-2	1.488	1.823	0.985	2.493	1.427	2.343

Natural charges (a.u.)								
	N	**C1**	**C2**	**O1**	**O2**	**H1**	**C3**	**NH$_3$**
COR-0	-1.17	0.23	0.22	-0.51	-0.49	0.40	-0.06	-0.01
COR-TS$_{0-1}$	-1.18	0.19	0.16	-0.65	-0.48	0.42	0.12	0.00
COR-1	-1.17	-0.01	0.22	-0.52	-0.52	0.40	0.18	0.00
COR-TS$_{1-2}$	-0.99	0.16	0.20	-0.69	-0.52	0.46	0.12	0.32
COR-2	-0.92	0.08	0.25	-0.76	-0.52	0.52	-0.01	-

Table S8: Atomic distances and natural charges for the ovalene model in Figure 8

Calculated atomic distances (Å) and natural atomic charges (a.u.) at each step of the ammonia addition mechanism on an ovalene based PRGO model. Atomic labels are used according to Figure 2. [a]Values from Ref 26 (Tang, S.; Cao, Z. Adsorption and Dissociation of Ammonia on Graphene Oxides: A First-Principles Study. J. Phys. Chem. C 2012, 116 (15), 8778–8791.)

Atomic distances (Å)									
	N-C1		**N-H1**		**O1-H1**		**O1-C1**	**O1-C2**	**O1-C3**
0	4.245		1.020		2.342		1.441	1.443	2.461
TS$_{0-1}$	5.005		1.028		1.966		2.275	1.389	2.230
1	3.808		1.020		2.314	2.22[a]	2.491	1.444	1.483
TS$_{1-2}$	2.212	3.35[a]	1.031		1.806	2.13[a]	2.480	1.385	2.019
2	1.488	1.49[a]	1.815	1.59[a]	0.986	1.02[a]	2.489	1.430	2.339

Natural charges (a.u.)									
	N	**C1**	**C2**	**O1**	**O2**	**H1**	**C3**	**NH$_3$**	
0	-1.17	0.24	0.22	-0.51	-0.49	0.40	0.00	0.00	
TS$_{0-1}$	-1.18	0.17	0.16	-0.68	-0.49	0.42	0.20	0.00	
1	-1.17	-0.02	0.23	-0.52	-0.51	0.40	0.23	0.00	
TS$_{1-2}$	-1.03	0.18	0.20	-0.69	-0.52	0.46	0.15	0.25	0.39[a]
2	-0.92	0.08	0.24	-0.77	-0.52	0.52	0.02	-	

Table S9: Calculated NPA natural charges and atom-atom overlap-weighted NAO bond orders of carbon atoms in structure 1

Carbon atoms	The role of C within structure	Natural charges (a.u.)	Bond orders (a.u.)
C(1)	Edges	-0.20	3.12
C(2)	Edges	-0.08	3.40
C(3)	Inner, sp2	0.05	3.30
C(4)	Inner, sp2	-0.01	3.37
C(5)	Edges	-0.07	3.37
C(6)	Edges	-0.20	3.11
C(7)	Inner, sp3	0.22	3.46
C(8)	Inner, sp3	0.22	3.42
C(9)	**Inner, sp3 (C2)**	**0.23**	**3.49**
C(10)	**Inner, sp3 (C3)**	**0.23**	**3.48**
C(11)	**Inner, sp2 (C1)**	**-0.02**	**3.23**
C(12)	Inner, sp3	0.22	3.41
C(13)	Inner, sp3	0.23	3.44
C(14)	Inner, sp3	0.24	3.44
C(15)	Edges, sp3	0.18	3.39
C(16)	Edges	-0.18	3.03
C(17)	Edges	-0.22	3.14
C(18)	Edges	-0.03	3.26
C(19)	Edges	-0.08	3.33
C(20)	Edges	-0.18	3.10
C(21)	Edges	-0.22	3.12
C(22)	Edges	-0.04	3.40
C(23)	Edges	-0.21	3.12
C(24)	Edges	-0.18	3.05
C(25)	Edges	-0.15	3.12
C(26)	Edges	-0.08	3.32
C(27)	Edges	-0.06	3.33
C(28)	Edges	-0.16	3.11
C(29)	Edges	-0.20	3.10
C(30)	Edges	-0.21	3.11
C(31)	Edges	-0.21	3.10
C(32)	Edges	-0.20	3.10

5. Ammonia addition on the PRGO models in the presence of water molecules

Table S10: The results of calculations in the case of one water molecule approximating the opposite side of the plane of the ovalene model.

Notation	ΔE [kcal/mol]
0-H2O-o	0
$TS_{0\text{-}1}$-H2O-o	34.4
1-H2O-o	11.2
1'-H2O-o	13.5
$TS_{1'\text{-}2}$-H2O-o	36.6
2-H2O-o	-5.8

Table S11: Atomic distances and natural charges for the one water-one ammonia ovalene model in Figure 11

Calculated atomic distances (Å) and natural atomic charges (a.u.) at each step of the water-assisted ammonia addition mechanism on an ovalene based PRGO model. Atomic labels are used according to Figure 10a.

Atomic distances (Å)							
	N-C1	**N-H1**	**O1-C1**	**O1-C2**	**O1-C3**	**O5-H1**	**O1-H4**
0-H_2O	3.670	1.023	1.444	1.447	2.463	2.252	1.946
$TS_{0\text{-}1}$-H_2O	3.523	1.022	2.302	1.393	2.262	2.290	1.733
1-H_2O	3.848	1.024	2.494	1.445	1.476	2.151	1.917
$TS_{1\text{-}2}$-H_2O	2.368	1.023	2.480	1.386	2.072	2.020	1.717
2-H_2O	1.534	1.052	2.463	1.367	2.333	1.748	1.594
$TS_{2\text{-}3}$-H_2O	1.528	1.117	2.483	1.390	2.348	1.483	1.239
3-H_2O	1.494	1.872	2.508	1.431	2.372	0.994	0.985

Natural charges (a.u.)									
	N	**H1**	**C1**	**C2**	**C3**	**O1**	**O5**	**H4**	**NH3**
0-H_2O	-1.18	0.41	0.24	0.22	-0.01	-0.53	-1.01	0.51	0.00
$TS_{0\text{-}1}$-H_2O	-1.19	0.41	0.20	0.18	0.16	-0.73	-1.04	0.52	0.00
1-H_2O	-1.18	0.41	-0.02	0.23	0.23	-0.54	-1.01	0.51	-0.01
$TS_{1\text{-}2}$-H_2O	-1.05	0.44	0.20	0.20	0.15	-0.72	-1.05	0.52	0.16
2-H_2O	-0.83	0.50	0.10	0.25	0.04	-0.88	-1.06	0.53	0.43
$TS_{2\text{-}3}$-H_2O	-0.85	0.50	0.10	0.25	0.03	-0.85	-1.10	0.52	0.42
3-H_2O	-0.93	0.52	0.09	0.27	-0.01	-0.78	-1.03	0.53	-

6. Interaction of two ammonia molecules with PRGO models

Figure S4: Labelling the atomic positions in two ammonia structures represented on the balls and sticks image of structure $TS_{1\text{-}2}$-$2NH_3$. (red=O, orange=C, white=H, blue=N)

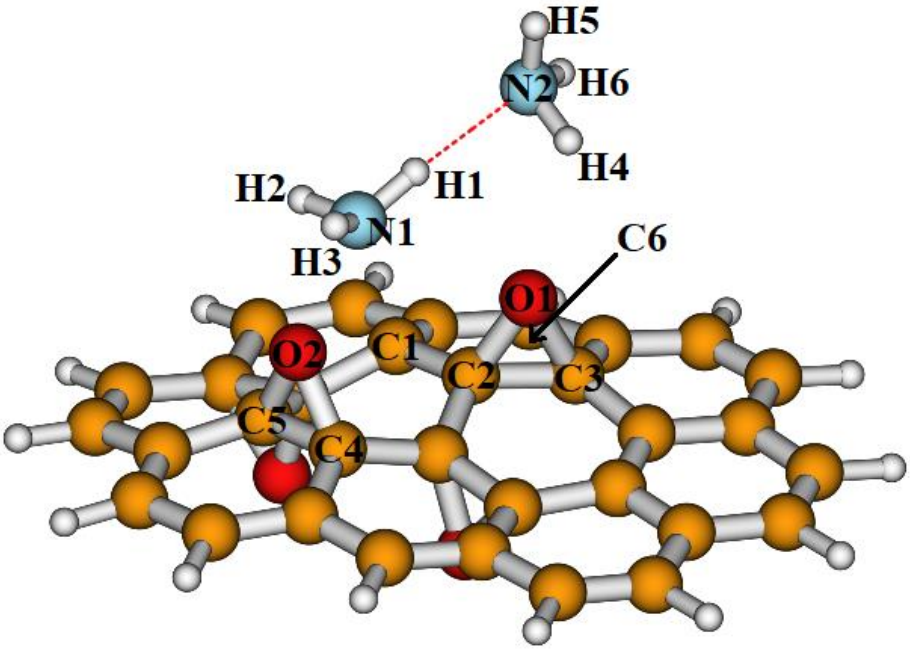


Table S12: Atomic distances and natural charges for the two ammonia ovalene models in Figure 13.

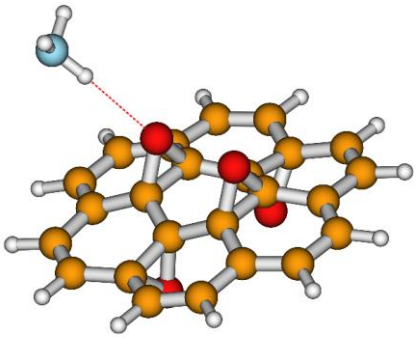
Calculated atomic distances (Å) and natural atomic charges (a.u.) at each step of the ammonia addition mechanism with two ammonia molecules on an ovalene based PRGO model. Atomic labels are used according to Figure 2.

Atomic distances (Å)									
	NH_3-NH_3		NH_3-epoxy						
	H1-N1	H1-N2	H3-N1	H3-O1	H4-O1	H4-N2	H2-O2	H5-O2	N1-C1
0-$2NH_3$	1.028	2.196	1.020	5.914	2.247	1.021	5.878	2.982	4.912
$TS_{0\text{-}1}$-$2NH_3$	1.031	2.154	1.020	6.080	2.014	1.029	5.677	2.845	4.810
1-$2NH_3$	1.028	2.203	1.020	6.721	2.791	1.020	5.800	2.273	4.917
$TS_{1\text{-}2}$-$2NH_3$	1.038	1.956	1.020	2.844	2.307	1.021	3.283	5.739	1.916
2-$2NH_3$	1.023	2.146	1.751	0.994	5.388	1.019	2.206	5.928	1.482

Natural charges (a.u.)													
	NH_3		NH_3-epoxy										
	NH_3-1	NH_3-2	O1	O2	C1	C2	C3	N1	N2	H1	H2	H3	H4
0-$2NH_3$	-0.01	0.02	-0.52	-0.51	0.24	0.22	-0.01	-1.19	-1.18	0.42	0.38	0.38	0.41
$TS_{0\text{-}1}$-$2NH_3$	-0.01	0.01	-0.68	-0.49	0.19	0.16	0.17	-1.19	-1.19	0.42	0.38	0.38	0.43
1-$2NH_3$	-0.01	0.02	-0.52	-0.53	-0.02	0.23	0.23	-1.19	-1.18	0.42	0.38	0.38	0.40
$TS_{1\text{-}2}$-$2NH_3$	0.39	0.04	-0.57	-0.54	0.13	0.22	0.23	-0.95	-1.18	0.46	0.43	0.45	0.42
2-$2NH_3$	-	0.03	-0.77	-0.52	0.08	0.25	0.04	-0.94	-1.17	0.44	0.42	0.52	0.40

7. XYZ Coordinates of optimised structures

Coordinates of Figure 8



CO-0

Energy=-1279.0418915

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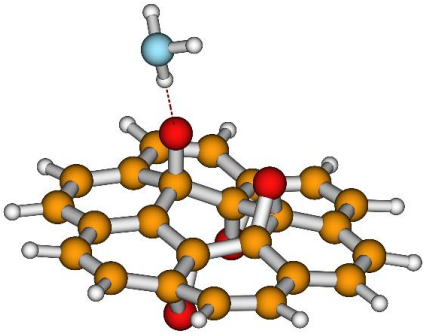
C	0.090488	1.396641	-0.222787
C	-1.233288	1.023774	0.376444
C	-2.337566	1.995665	0.241791
C	-1.971397	3.392331	0.087377
C	-1.558534	-0.446660	0.416413
C	-0.521353	-1.372930	-0.146640
C	0.927069	-1.007149	-0.007563
C	1.251220	0.462255	-0.049923
C	1.792285	3.240353	-0.610354
C	2.782267	2.319086	-0.716091
C	2.557287	0.890068	-0.590833
C	3.482934	-0.087392	-0.860586
C	3.172389	-1.490260	-0.823412
C	1.924771	-1.973106	-0.511786
C	-3.620898	1.516048	0.341282
C	-3.931224	0.113010	0.377791
C	-2.971006	-0.867482	0.317582
C	-3.229952	-2.294035	0.237043
C	-2.262405	-3.214360	-0.001976
C	-0.881188	-2.808564	-0.361114
C	0.239092	-3.779385	-0.423003
C	1.523864	-3.367823	-0.565241
O	1.309811	-0.287047	1.176999
O	-0.030169	1.868920	-1.561171
O	-1.213650	0.280863	1.604283
O	-0.843029	-1.817319	-1.461215
H	3.951084	-2.189408	-1.120727
H	4.482675	0.202906	-1.174862
H	2.309381	-4.107074	-0.710346
H	-0.004201	-4.838858	-0.415409
H	-2.496198	-4.275974	0.002643
H	-4.254506	-2.624971	0.396400
H	-4.980576	-0.174487	0.383207
H	-4.451024	2.219089	0.321305
H	-2.758550	4.132087	0.220734
H	-0.472706	4.865040	-0.238155
H	2.018776	4.302603	-0.654712
H	3.805759	2.649020	-0.882344
H	3.221915	-0.264553	2.468108
N	4.065305	-0.186547	3.036923
H	3.853309	0.453278	3.801049
H	4.232039	-1.101068	3.454113



CO-TS$_{0\text{-}1}$

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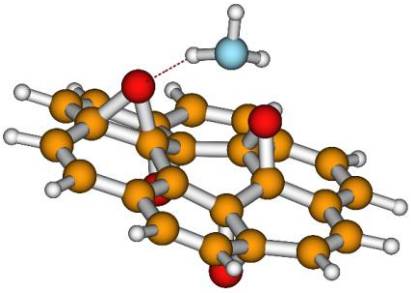
C	-0.831094	1.168337	-0.372398
C	-1.437396	-0.190660	-0.074691
C	-2.774348	-0.408400	-0.743001
C	-3.656309	0.733922	-0.791570
C	-0.468019	-1.297660	-0.314199
C	0.978271	-1.009196	-0.225495
C	1.449199	0.292752	0.337278
C	0.496868	1.449863	0.252177
C	-1.218064	3.672918	-0.368356
C	0.086468	3.885614	-0.066111
C	1.044398	2.817057	0.145683
C	2.400011	2.978867	0.307982
C	3.310033	1.869788	0.419790
C	2.903499	0.556590	0.352133
C	-3.147876	-1.698598	-1.097407
C	-2.228300	-2.758766	-1.035802
C	-0.885750	-2.593760	-0.640433
C	0.067091	-3.700276	-0.543334
C	1.383013	-3.513563	-0.300122
C	1.963921	-2.154403	-0.279649
C	3.334368	-1.874409	0.221772
C	3.772506	-0.603089	0.419050
O	0.740900	0.763084	1.490440
O	-0.959278	1.604084	-1.721689
O	-1.707261	-0.428116	1.266527
O	1.629221	-1.356900	-1.458771
H	4.373452	2.092824	0.509309
H	2.821370	3.979794	0.298937
H	4.814277	-0.431293	0.682916
H	4.002884	-2.716945	0.362205
H	2.044621	-4.350612	-0.133312
H	-0.329690	-4.719655	-0.621568
H	-2.566969	-3.755637	-1.309250
H	-4.165870	-1.896193	-1.425389

H	-4.724878	0.563085	-0.908330
H	-3.872282	2.841354	-0.716495
H	-1.906513	4.516129	-0.468816
H	0.446808	4.898681	0.041022
H	-1.539839	-1.391461	3.133590
N	-1.590780	-1.836256	4.052649
H	-0.901689	-1.382190	4.652171
H	-2.510477	-1.617646	4.436705



CO-1

Energy=-1279.0364273

C	-3.783602	-0.390733	-0.366031
C	-2.800081	0.732199	-0.448270
C	-1.372554	0.401067	-0.299933
C	-0.941427	-0.996483	0.036369
C	-1.983974	-2.074497	0.024485
C	-3.406083	-1.669132	-0.207131
C	0.442576	-1.326990	-0.337761
C	1.372277	-0.220129	-0.598107
C	1.038854	1.115064	-0.010087
C	-0.412950	1.453737	0.143781
C	-3.190099	2.136453	-0.159119
C	-2.264957	3.112455	0.027844
C	-0.835024	2.862993	0.079884
C	0.150559	3.819374	0.082409
C	1.550479	3.498184	-0.005953
C	2.017780	2.212826	-0.136305
C	-1.499557	-3.424469	-0.329732
C	-0.177607	-3.676866	-0.495499
C	0.837421	-2.627375	-0.500025
C	2.254850	-2.923716	-0.678542
C	3.204294	-1.959166	-0.749589
C	2.842784	-0.529537	-0.814647
C	3.810573	0.550465	-0.496550
C	3.410834	1.827413	-0.271953
O	0.381198	1.040965	1.274697
O	-1.889492	0.600713	-1.617662
O	-1.438147	-1.532156	1.274872
N	1.095334	-1.440170	3.389927
O	1.942747	-0.166972	-1.909354
H	2.259746	4.322914	-0.026772
H	-0.129294	4.870881	0.089170
H	4.159308	2.606592	-0.141517
H	4.868371	0.298850	-0.503657
H	4.259530	-2.221724	-0.739648
H	2.554736	-3.969390	-0.674952
H	0.147847	-4.692172	-0.712009
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H	-4.150523	-2.462971	-0.214250
H	-4.835719	-0.140822	-0.485977
H	-4.249786	2.379261	-0.153878
H	-2.596570	4.141948	0.149906
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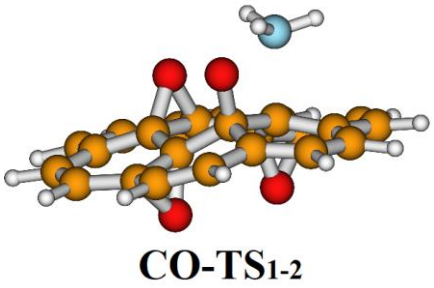

CO-TS$_{1-2}$

Energy=-1278.9934228

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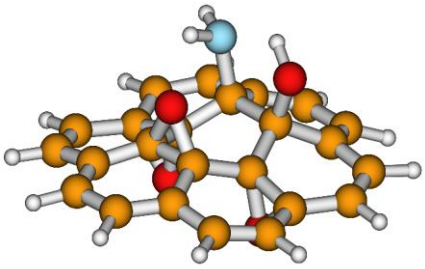
C	-2.764136	0.712796	-0.437526
C	-1.364181	0.376873	-0.095280
C	-1.041597	-1.028212	0.421373
C	-1.997984	-2.068647	-0.071522
C	-3.392764	-1.670164	-0.240226
C	0.461029	-1.356511	0.210697
C	1.356666	-0.235035	-0.207373
C	1.018198	1.146653	0.260457
C	-0.447682	1.481593	0.320154
C	-3.177193	2.131974	-0.307634
C	-2.274093	3.124096	-0.114528
C	-0.857843	2.877436	0.079848
C	0.124058	3.838282	0.045300
C	1.523848	3.519305	0.024703
C	1.991476	2.227238	0.016619
C	-1.542595	-3.368787	-0.328247
C	-0.175959	-3.631586	-0.408056
C	0.827709	-2.659784	-0.224009
C	2.242015	-2.940948	-0.413108
C	3.189009	-1.970386	-0.459540
C	2.790070	-0.545922	-0.523837
C	3.770807	0.552501	-0.339174
C	3.378473	1.838033	-0.156472
O	0.309420	1.223080	1.515166
O	-1.724759	0.479758	-1.475995
O	-1.531537	-1.311056	1.690888
N	1.014139	-1.384003	2.205348
O	1.788580	-0.259115	-1.568805
H	2.231537	4.338862	-0.081864
H	-0.161114	4.882204	-0.067790
H	4.127156	2.627390	-0.121851
H	4.826701	0.303529	-0.412241
H	4.245492	-2.215063	-0.533506
H	2.540989	-3.985295	-0.493610
H	0.141181	-4.636739	-0.684185
H	-2.260807	-4.162928	-0.512973
H	-4.136708	-2.463472	-0.272246

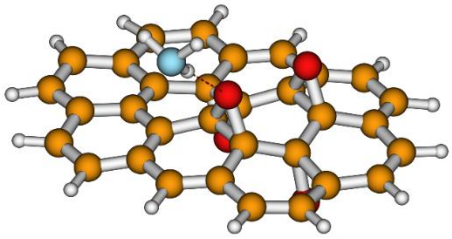
H	-4.815414	-0.120080	-0.504605
H	-4.233428	2.365163	-0.418139
H	-2.607548	4.160135	-0.109876
H	1.649835	-2.164298	2.339517
H	1.353870	-0.529117	2.638562
H	0.044489	-1.576075	2.504941



CO-2

Energy=-1279.0547565

C	-3.742103	-0.398272	-0.344369
C	-2.737575	0.692340	-0.380880
C	-1.335311	0.353915	-0.011415
C	-1.057066	-1.035044	0.570914
C	-1.949309	-2.065203	-0.122426
C	-3.347058	-1.686618	-0.281035
C	0.529916	-1.382201	0.574420
C	1.362382	-0.265041	-0.086416
C	1.046623	1.141993	0.322516
C	-0.423605	1.470858	0.392362
C	-3.153445	2.110213	-0.267218
C	-2.254617	3.105480	-0.078705
C	-0.839675	2.859917	0.119051
C	0.137164	3.824626	0.051387



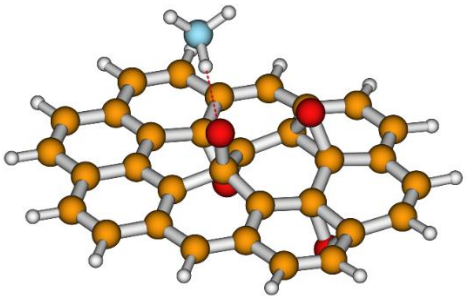
0

Energy=-1585.1684003

C	-2.650910	-0.557145	-0.252539
C	-1.436005	-1.297572	-0.219627
C	-0.189414	-0.620581	0.166380
C	-0.126151	0.863344	-0.033503
C	-1.396915	1.618172	-0.170238
C	-2.669693	0.863458	-0.121539
C	1.100004	-1.368766	0.075546
C	2.321387	-0.549733	-0.224420
C	2.398394	0.854477	0.302680
C	1.097169	1.604911	0.406264
C	3.636362	1.612645	0.040926
C	4.846677	0.842725	-0.168908
C	4.851256	-0.500093	-0.373720
C	3.590810	-1.256979	-0.568648
C	1.534037	3.508482	-0.005015
C	2.002182	2.216100	0.002189
C	-1.477977	-3.291376	-0.455040
C	-0.068019	-3.603954	-0.445790
C	0.888209	-2.712522	-0.086564
C	2.308825	-2.973432	-0.285058
C	3.214360	-1.978477	-0.417634
C	2.765717	-0.566017	-0.494206
C	3.750579	0.541032	-0.453516
C	3.371484	1.829114	-0.270193
O	0.354463	1.262469	1.582628
O	-1.675388	0.442903	-1.390663
O	-1.534833	-0.985577	1.914933
N	0.929940	-1.510870	2.001702
O	1.662242	-0.369658	-1.471092
H	2.235709	4.323751	-0.168954
H	-0.155607	4.864091	-0.081026
H	4.114431	2.622338	-0.329414
H	4.795566	0.293448	-0.623753
H	4.270608	-2.191769	-0.561647
H	2.625873	-4.011692	-0.368835
H	0.240004	-4.568351	-0.846358
H	-2.165802	-4.045242	-0.833143
H	-4.079675	-2.486514	-0.372107
H	-4.791579	-0.132915	-0.443323
H	-4.210533	2.337394	-0.381284
H	-2.587237	4.141710	-0.084485
H	1.760303	-2.090435	2.088676
H	1.126375	-0.596153	2.403964
H	-0.834312	-1.422881	2.452627

C	1.081843	-2.775234	-0.392640
C	2.375404	-3.420501	-0.565209
C	3.548423	-2.742208	-0.583808
C	1.092361	3.074428	0.240797
C	2.322221	3.701654	0.185927
C	3.559260	2.987777	0.087466
C	-0.183906	3.737731	0.219829
C	-1.388972	3.079095	0.120938
C	-1.402000	-2.679026	-0.448085
C	-0.131556	-3.383841	-0.541193
O	2.710092	-0.644509	-1.591834
O	1.774932	1.115962	1.570655
O	-0.563768	1.253984	-1.334830
O	0.456666	-1.145483	1.345561
N	-0.454912	-3.808395	3.181816
C	-2.644306	-3.352963	-0.648199
H	-0.168320	-4.442150	-0.791802
C	-3.884797	-1.262064	-0.403906
C	-3.870778	1.568022	-0.053519
C	-2.676518	3.721112	0.189800
H	-0.186525	4.824231	0.297301
H	2.357424	4.788273	0.145324
H	4.472187	3.569430	-0.023246
H	5.792514	1.380331	-0.136266
H	5.789710	-1.041406	-0.462503

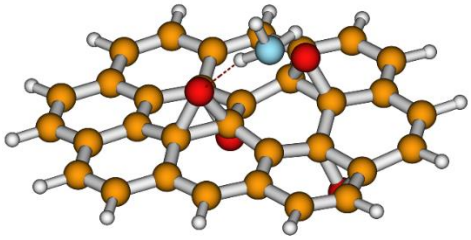
H	4.491777	-3.275650	-0.669717
H	2.381693	-4.503886	-0.666404
H	-0.164416	-2.979683	2.662432
H	0.046734	-3.798917	4.068694
H	-1.443711	-3.692504	3.399139
C	-3.840081	-2.671940	-0.602083
C	-3.839540	3.015481	0.097917
C	-5.098971	-0.522038	-0.342908
C	-5.094641	0.841847	-0.152022
H	-6.034593	1.386467	-0.099931
H	-6.042093	-1.053506	-0.448444
H	-4.791314	3.538684	0.152358
H	-2.705241	4.800283	0.323464
H	-4.776382	-3.211543	-0.725367
H	-2.636928	-4.426493	-0.820694



TS_{0-1}

Energy=-1585.1145333

O	0.192701	0.847098	1.759516
C	-1.186582	1.486898	0.067609
C	-1.252087	2.877801	-0.008028
C	-0.031212	3.590795	-0.069912
C	1.235856	2.974270	-0.086102
C	1.310194	1.557715	-0.034674
C	-2.557246	3.538943	0.031302
C	-3.725574	2.858244	-0.000991
C	-3.746606	1.399106	-0.249358
C	-2.405737	0.690739	-0.154214
C	-2.414395	-0.768215	0.176647
C	-3.646362	-1.534107	-0.089601
C	-4.891110	-0.793952	-0.053674
C	-4.951957	0.563236	-0.027270
C	0.098715	0.772798	0.375960
C	0.091489	-0.638427	-0.180990
C	-1.091454	-1.478138	0.161083
C	-1.051127	-2.912823	-0.188715
C	-2.261197	-3.573187	-0.283284
C	-3.523908	-2.900311	-0.221312
C	0.244782	-3.510809	-0.367670
C	1.419241	-2.795294	-0.402405
C	1.370841	-1.308355	-0.439607
C	2.619064	-0.528122	-0.274912
C	2.558029	0.889916	-0.156272
O	-2.992744	0.994848	-1.432011
O	-1.739757	-1.123953	1.392389
O	0.515809	-0.772197	-1.539479
N	1.613317	-1.484216	2.963436
C	2.460858	3.726452	-0.147619
H	-0.071498	4.678863	-0.110965
C	3.761241	1.659904	-0.185418
C	3.844456	-1.192931	-0.344403
C	2.727089	-3.393147	-0.472972
H	0.290112	-4.594928	-0.462146
H	-2.264122	-4.644471	-0.473163
H	-4.424646	-3.499944	-0.336530
H	-5.813804	-1.368737	0.001440
H	-5.904399	1.073267	0.092055
H	-4.673997	3.370713	0.138366
H	-2.566907	4.620452	0.150020
H	1.116438	-0.636922	2.658472
H	2.313781	-1.188919	3.643362
H	0.937659	-2.052744	3.473955
C	3.672528	3.092727	-0.164181
C	3.864304	-2.643423	-0.456200
C	4.994083	0.967927	-0.259325
C	5.033332	-0.413070	-0.316680
H	2.407756	4.812508	-0.164884
H	4.593413	3.670103	-0.186881
H	5.920385	1.537376	-0.273613
H	5.993926	-0.921303	-0.366138
H	4.833753	-3.133648	-0.505400
H	2.793560	-4.477498	-0.526206

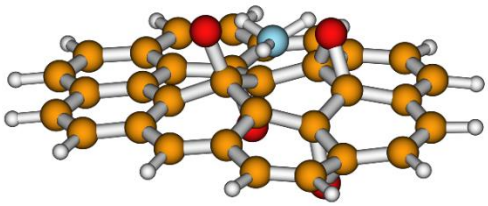


1

Energy=-1585.1514947

C	4.773706	0.967343	-0.246238
C	3.526107	1.691617	-0.103882
C	2.307830	0.876053	0.057793
C	2.282614	-0.509303	-0.512666
C	3.626681	-1.185903	-0.732430
C	4.837133	-0.379261	-0.441507
C	0.994585	1.571712	0.243793
C	-0.208263	0.790445	-0.155117
C	-0.126429	-0.668259	0.173181
C	1.116314	-1.341471	-0.213805
C	-1.409385	-1.453127	0.161968
C	-2.702793	-0.742366	-0.061153
C	-2.757150	0.657748	-0.099139
C	-1.510897	1.464148	-0.223991
C	0.927164	3.042691	0.169066
C	-0.380549	3.643648	0.141216
C	-1.557254	2.933109	0.028179
C	1.164263	-2.709996	-0.340064
C	-0.067444	-3.476646	-0.284000
C	-1.310256	-2.903374	-0.148193
C	2.464517	-3.350345	-0.522469

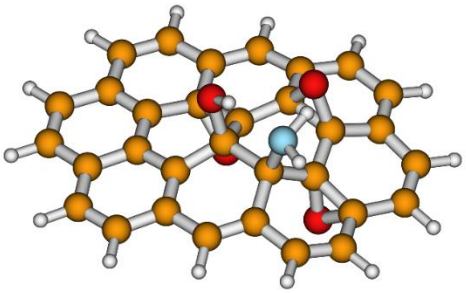
C	3.613934	-2.659479	-0.633581
C	3.394929	3.057871	0.016507
C	2.129361	3.720731	0.132682
O	-0.733164	1.113614	-1.444149
O	-0.739249	-1.052735	1.423088
O	2.833734	-0.628037	-1.827163
O	1.688135	0.981575	1.361704
N	1.656239	-1.909914	3.512281
H	4.288438	3.677162	-0.028823
H	2.123079	4.808687	0.133234
H	5.696424	1.535022	-0.140643
H	5.797089	-0.890199	-0.442230
H	4.568520	-3.179850	-0.630185
H	2.497783	-4.436695	-0.490240
H	-0.000968	-4.552842	-0.434779
C	-2.562854	-3.617256	-0.257618
C	-3.882988	-1.511841	-0.158937
C	-3.994877	1.333078	-0.122027
C	-2.868040	3.531155	0.027462
H	-0.433708	4.729999	0.202220
H	1.435397	-2.134154	4.481506
H	2.136498	-1.010831	3.517053
H	0.771933	-1.756290	3.027729
C	-3.776706	-2.962284	-0.227224
C	-4.005633	2.785350	-0.070252
C	-5.119879	-0.829747	-0.217954
C	-5.176195	0.557974	-0.171704
H	-2.529444	-4.699235	-0.371883
H	-4.699929	-3.533300	-0.304627
H	-6.039516	-1.405836	-0.293140
H	-6.140355	1.061076	-0.191591
H	-4.972484	3.283245	-0.079052
H	-2.937361	4.614018	0.104262



TS_{1-2}

Energy=-1585.1142351

C	4.745164	0.905613	-0.356903
C	3.522282	1.644701	-0.121745
C	2.317893	0.860141	0.201612
C	2.253114	-0.565675	-0.254240
C	3.538507	-1.245445	-0.634174
C	4.780280	-0.441975	-0.521068
C	1.000772	1.571615	0.348949
C	-0.196598	0.747602	0.018711
C	-0.219348	-0.694305	0.529624
C	1.115599	-1.401725	0.209193
C	-1.432655	-1.443887	0.068449
C	-2.686146	-0.750825	-0.053507
C	-2.738261	0.662091	-0.096129
C	-1.478418	1.438143	-0.206622
C	0.948242	3.026522	0.105593
C	-0.348806	3.634925	0.003294
C	-1.523118	2.923222	-0.075888
C	1.113093	-2.768308	-0.157151
C	-0.106820	-3.460137	-0.226571
C	-1.371505	-2.850183	-0.117273
C	2.397617	-3.416091	-0.402297
C	3.552813	-2.724037	-0.542657
C	3.407820	3.018122	-0.112285
C	2.152421	3.694869	-0.010003
O	-0.630791	0.959215	-1.328864
O	-0.668367	-0.828584	1.833321
O	2.596634	-0.723871	-1.636425
O	1.739200	1.125594	1.496236
N	1.824185	-1.559347	2.298265
H	4.299171	3.621198	-0.273423
H	2.145746	4.777149	-0.120566
H	5.674872	1.471311	-0.381147
H	5.729203	-0.960143	-0.634815
H	4.504796	-3.237509	-0.652564
H	2.412525	-4.504091	-0.443318
H	-0.074864	-4.528710	-0.440083
C	-2.603673	-3.582304	-0.226691
C	-3.887488	-1.508014	-0.144102
C	-3.960733	1.340278	-0.137063
C	-2.826562	3.535335	-0.113105
H	-0.393860	4.722919	-0.022261
H	2.175353	-2.497391	2.465130
H	2.423296	-0.850042	2.711358
H	0.848155	-1.431603	2.605733
C	-3.810995	-2.941987	-0.204351
C	-3.968974	2.793966	-0.153968
C	-5.118758	-0.806651	-0.195341
C	-5.156334	0.573637	-0.170112
H	-2.558407	-4.665010	-0.322958
H	-4.735950	-3.509524	-0.270055
H	-6.044952	-1.373753	-0.254433
H	-6.113046	1.090535	-0.199486
H	-4.934327	3.294290	-0.182274
H	-2.882974	4.621578	-0.099913



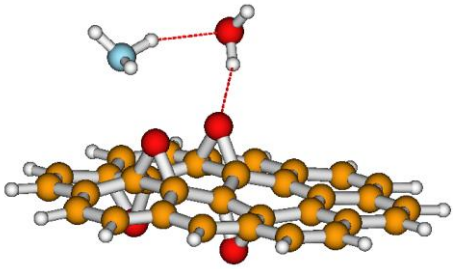
2

Energy=-1585.1817851

C	4.692610	0.923410	-0.569729
C	3.498747	1.658243	-0.212413
C	2.329937	0.878940	0.224189
C	2.241206	-0.575653	-0.132500
C	3.482548	-1.242532	-0.618977
C	4.715527	-0.425363	-0.712753

C	1.006480	1.580791	0.383232
C	-0.185906	0.729267	0.089120
C	-0.236856	-0.675523	0.694639
C	1.204968	-1.413327	0.640628
C	-1.394819	-1.458929	0.087981
C	-2.642181	-0.789384	-0.068032
C	-2.725082	0.631095	-0.070215
C	-1.473510	1.413518	-0.173939
C	0.932528	3.024619	0.080282
C	-0.368577	3.622546	-0.019397
C	-1.534933	2.898517	-0.074898
C	1.162524	-2.822572	0.054013
C	-0.004808	-3.472169	-0.154130
C	-1.310414	-2.830086	-0.113196
C	2.455175	-3.444080	-0.222358
C	3.563511	-2.718915	-0.488266
C	3.377053	3.031078	-0.242174
C	2.124890	3.701194	-0.095099
O	-0.605654	0.900203	-1.260953
O	-0.611447	-0.474596	2.059735
O	2.387982	-0.805321	-1.526981
O	1.793569	1.211076	1.524878
N	1.656952	-1.576318	2.049138
H	4.250326	3.631192	-0.489831
H	2.101305	4.778836	-0.241902
H	5.604517	1.495749	-0.729775
H	5.644378	-0.937979	-0.950539
H	4.516052	-3.201072	-0.693728
H	2.496558	-4.531588	-0.254653
H	0.025310	-4.510497	-0.483493
C	-2.499670	-3.576307	-0.363063
C	-3.837593	-1.550879	-0.254274
C	-3.950668	1.289052	-0.134837
C	-2.845360	3.497113	-0.109347
H	-0.421189	4.709356	-0.067920
H	2.307228	-2.353141	2.128780
H	2.113191	-0.729076	2.381860
H	0.008140	-1.036125	2.582235
C	-3.730333	-2.961963	-0.388668
C	-3.979071	2.743697	-0.146813
C	-5.082832	-0.862149	-0.310716
C	-5.142114	0.509433	-0.224790
H	-2.422766	-4.651064	-0.512373
H	-4.634183	-3.548729	-0.535667
H	-5.995852	-1.441407	-0.429140
H	-6.102664	1.018017	-0.265438
H	-4.950422	3.231966	-0.177768
H	-2.912046	4.582805	-0.099039

Coordinates of Figure 11

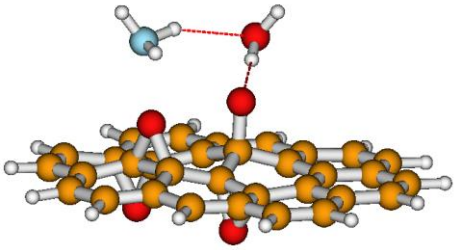


0-H_2O

Energy=-1661.602300

C	4.524799	1.377452	-0.618983
C	3.259197	2.009211	-0.300463
C	2.132212	1.117978	0.035694
C	2.169325	-0.279833	-0.511013
C	3.471864	-0.840061	-0.959364
C	4.654702	0.046086	-0.847037
C	0.769789	1.722638	0.245079
C	0.594914	3.185129	0.113884
C	1.743164	3.941734	-0.018076
C	3.038829	3.367071	-0.221880
C	1.065117	-1.227322	-0.144097
C	-0.289119	-0.624886	0.044971
C	-0.398159	0.860441	-0.121836
C	-1.748771	1.475392	-0.146571
C	-1.874813	2.923561	0.177906
C	-0.742643	3.706780	0.203214
C	-2.927077	0.587486	-0.023389
C	-2.767342	-0.820549	-0.188901
C	-1.481809	-1.426713	-0.261008
C	-1.317093	-2.792792	-0.521726
C	0.012276	-3.355199	-0.715714
C	1.163279	-2.623794	-0.635369
C	2.501853	-3.122273	-0.918056
C	3.587630	-2.319320	-1.005432
C	-4.188058	1.157195	0.147812
C	-4.300207	2.597003	0.330680
C	-3.214764	3.421762	0.354601
C	-3.926958	-1.651979	-0.267255
C	-5.205098	-1.048467	-0.101257
C	-5.331604	0.304671	0.121331
C	-2.492283	-3.592859	-0.649941
C	-3.747035	-3.045116	-0.502634
O	1.578344	1.296183	1.351154
O	-0.970902	1.221480	-1.377919
O	0.491451	-1.084162	1.173208
O	2.455067	-0.312940	-1.907419
N	3.510200	-1.142774	2.591744
O	1.031420	-3.100094	3.171709
H	0.070450	-4.405212	-0.996878
H	-0.855198	4.785361	0.306064
H	1.658944	5.026306	-0.038257
H	3.872832	4.045368	-0.390085
H	5.407448	2.013595	-0.647305
H	5.635740	-0.392926	-1.008028
H	4.575783	-2.744855	-1.159088
H	2.617530	-4.197105	-1.040764
H	2.974264	-0.286818	2.734529
H	4.330208	-1.086093	3.194342
H	2.928601	-1.908995	2.938440
H	-2.384754	-4.656131	-0.850903
H	-4.627127	-3.680416	-0.572592

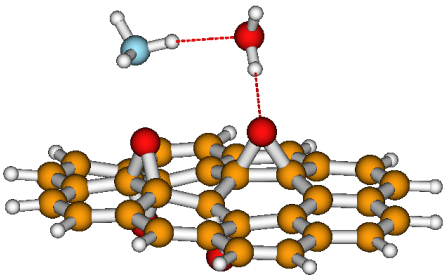
H	-6.091550	-1.676792	-0.150603
H	-6.317627	0.743842	0.254342
H	-5.295488	3.013731	0.465827
H	-3.348007	4.489436	0.514982
H	0.666764	-2.514971	2.480384
H	0.510061	-2.914209	3.966477



$TS_{0\text{-}1}$-H_2O

Energy=-1661.555713

C	4.654756	1.233110	-0.397978
C	3.392227	1.915407	-0.195605
C	2.212820	1.063446	0.045112
C	2.216805	-0.321474	-0.517928
C	3.554085	-0.947223	-0.844335
C	4.751205	-0.105452	-0.600557
C	0.871410	1.708988	0.252259
C	0.759615	3.177831	0.146137
C	1.936699	3.896166	0.064314
C	3.219734	3.278191	-0.090196
C	1.045222	-1.193179	-0.331184
C	-0.236992	-0.596544	0.186459
C	-0.310469	0.884951	-0.133122
C	-1.625892	1.537042	-0.191260
C	-1.716578	2.994086	0.103539
C	-0.563070	3.742280	0.174466
C	-2.836986	0.691293	-0.072455
C	-2.725078	-0.723634	-0.203764
C	-1.454505	-1.348417	-0.279934
C	-1.342490	-2.729654	-0.557649
C	-0.053350	-3.292873	-0.703329
C	1.146366	-2.549615	-0.635879
C	2.466083	-3.155894	-0.814069
C	3.601370	-2.425726	-0.836000
C	-4.082179	1.305037	0.062257
C	-4.154911	2.752201	0.203489
C	-3.043689	3.540611	0.230446
C	-3.904070	-1.527788	-0.282106
C	-5.160486	-0.884242	-0.149065
C	-5.244214	0.481394	0.038223
C	-2.540525	-3.515060	-0.664012
C	-3.771601	-2.937686	-0.504069
O	1.635526	1.196007	1.351881
O	-0.841247	1.224494	-1.417678
O	-0.228145	-0.854024	1.555520
O	2.683449	-0.388615	-1.879516
N	2.948684	-1.493118	2.618647
O	0.354662	-3.355323	2.470436
H	0.016038	-4.362295	-0.896283
H	-0.647037	4.824345	0.267992
H	1.891363	4.983269	0.055122
H	4.088071	3.927272	-0.182613
H	5.562648	1.829579	-0.331845
H	5.723070	-0.589489	-0.646824
H	4.574783	-2.908351	-0.844730
H	2.516538	-4.241372	-0.854375
H	2.292464	-0.712833	2.666159
H	3.575015	-1.408541	3.418540
H	2.382155	-2.332046	2.760695
H	-2.453253	-4.581619	-0.856214
H	-4.673241	-3.542197	-0.562233
H	-6.067798	-1.481673	-0.196396
H	-6.219866	0.950480	0.145444
H	-5.139088	3.202747	0.307149
H	-3.145328	4.615444	0.363710
H	0.101357	-2.439247	2.172683
H	-0.220495	-3.547410	3.225121v

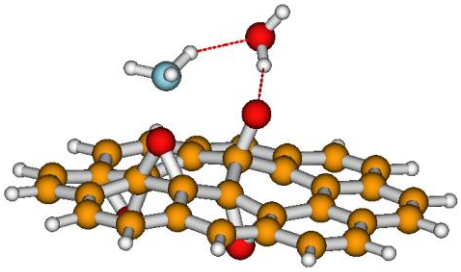


1-H_2O

Energy=-1661.586296

C	4.621189	1.262051	-0.443257
C	3.353186	1.923497	-0.209092
C	2.174712	1.050070	-0.050102
C	2.183928	-0.298280	-0.701016
C	3.540753	-0.901700	-1.009696
C	4.727850	-0.063655	-0.715566
C	0.842252	1.680767	0.215124
C	0.714050	3.149507	0.223067
C	1.887162	3.877538	0.184894
C	3.172770	3.275133	-0.009577
C	1.059498	-1.195099	-0.418235
C	-0.197448	-0.599183	0.043829
C	-0.341885	0.873641	-0.187573
C	-1.669459	1.497862	-0.181777
C	-1.765752	2.947604	0.152734
C	-0.615769	3.697305	0.268233
C	-2.877554	0.636429	-0.065599
C	-2.766057	-0.757293	-0.114999
C	-1.442341	-1.424554	0.015977
C	-1.303690	-2.845023	-0.387104
C	-0.048690	-3.360201	-0.603106
C	1.151474	-2.547812	-0.645446
C	2.465250	-3.125852	-0.916105
C	3.590004	-2.377281	-1.009089
C	-4.140857	1.259000	-0.010417
C	-4.209056	2.704370	0.123202
C	-3.097978	3.490374	0.225701
C	-3.914050	-1.569318	-0.220937

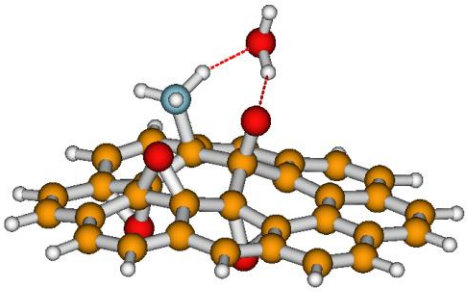
C	-5.178617	-0.938954	-0.198949
C	-5.289820	0.438303	-0.068855
C	-2.530329	-3.598579	-0.495758
C	-3.752182	-3.004858	-0.382744
O	1.594622	1.059935	1.275848
O	-0.917271	1.244069	-1.441458
O	-0.761778	-1.087389	1.281804
O	2.685064	-0.312183	-2.041468
N	3.513436	-1.336449	2.542122
O	0.760276	-2.798298	3.049687
H	0.050741	-4.421559	-0.823053
H	-0.709261	4.775598	0.391665
H	1.837816	4.962883	0.244309
H	4.038623	3.932520	-0.054284
H	5.524244	1.859951	-0.336450
H	5.704860	-0.537125	-0.768272
H	4.565195	-2.855240	-1.059283
H	2.538508	-4.210258	-0.957153
H	3.223946	-0.374252	2.715621
H	4.238924	-1.556194	3.223677
H	2.703629	-1.924081	2.758571
H	-2.460131	-4.668402	-0.678789
H	-4.653078	-3.608638	-0.463779
H	-6.075864	-1.548394	-0.279471
H	-6.273861	0.899868	-0.029309
H	-5.194938	3.160758	0.173076
H	-3.206887	4.563854	0.364519
H	0.230130	-2.268260	2.420687
H	0.380782	-2.611804	3.920978



$TS_{1\text{-}2}$-H_2O

Energy=-1661.554735

C	-5.137100	0.785625	-0.248436
C	-3.931257	1.530210	-0.138425
C	-2.718756	0.835683	-0.158798
C	-2.684313	-0.576556	-0.253888
C	-3.895895	-1.305400	-0.421591
C	-5.117858	-0.585789	-0.407930
C	-1.447615	1.599231	-0.193264
C	-0.177354	0.871158	-0.024336
C	-0.218340	-0.613405	0.352119
C	-1.442143	-1.291293	-0.204326
C	1.096252	-1.299119	-0.057108
C	2.253129	-0.445729	-0.411486
C	2.337884	0.933463	0.168762
C	1.030338	1.648862	0.375183
C	3.536805	-1.108824	-0.846391
C	4.788611	-0.337876	-0.646038
C	4.770246	0.991313	-0.368660
C	3.554860	1.725418	-0.083733
C	0.998768	3.119875	0.253282
C	2.212495	3.777941	0.195681
C	3.459035	3.094510	0.040795
C	1.085802	-2.624986	-0.522413
C	2.362672	-3.272436	-0.809851
C	3.527783	-2.588983	-0.885463
C	-0.289168	3.753815	0.204665
C	-1.472997	3.067646	0.066921
C	-1.399915	-2.674225	-0.509946
C	-0.143204	-3.295783	-0.649965
C	-2.639291	-3.379478	-0.692447
C	-3.837919	-2.727506	-0.617729
C	-3.920755	2.979621	-0.020671
C	-2.768262	3.698044	0.086077
O	1.762509	1.102235	1.480390
O	2.617386	-0.481896	-1.799869
O	-0.602067	1.207731	-1.349778
O	-0.641364	-0.839246	1.652021
N	1.961450	-1.665578	2.116051
H	4.359419	3.696469	-0.064340
H	2.221450	4.865672	0.176786
H	5.708002	1.542867	-0.333161
H	5.731363	-0.859547	-0.790997
H	4.474529	-3.106571	-1.019077
H	2.361060	-4.354351	-0.928370
H	-0.124787	-4.347547	-0.933559
H	-0.318697	4.840484	0.272875
H	2.957340	-1.869971	2.149397
H	1.756237	-0.802856	2.611243
H	1.414875	-2.429647	2.520752
H	-2.605406	-4.450102	-0.880413
H	-4.769979	-3.274132	-0.737916
H	-6.051091	-1.131843	-0.525149
H	-6.086764	1.315867	-0.230822
H	-4.879243	3.493311	-0.002576
H	-2.809685	4.779376	0.196840
H	-0.628486	-2.393115	2.383257
O	-0.400971	-3.266856	2.805590
H	-0.959454	-3.341230	3.592523

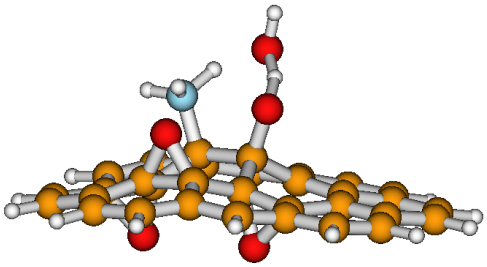


2-H_2O

Energy=-1661.591815

C	-5.123074	0.712477	-0.344461
C	-3.922380	1.463710	-0.173248
C	-2.706211	0.785347	-0.155582

C	-2.645558	-0.630930	-0.276464
C	-3.847879	-1.357121	-0.538079
C	-5.082568	-0.647557	-0.548518
C	-1.443338	1.558380	-0.175155
C	-0.172246	0.836912	0.038721
C	-0.263639	-0.610669	0.554236
C	-1.407582	-1.326425	-0.163253
C	1.176929	-1.353182	0.337503
C	2.248904	-0.472471	-0.317522
C	2.346178	0.946376	0.161347
C	1.032044	1.641924	0.402752
C	3.499790	-1.125730	-0.818841
C	4.739179	-0.314215	-0.830740
C	4.720152	1.022880	-0.594339
C	3.529595	1.741800	-0.199260
C	0.980641	3.109883	0.234433
C	2.182026	3.783266	0.110173
C	3.424301	3.113313	-0.103128
C	1.139261	-2.723130	-0.312775
C	2.431958	-3.338320	-0.592869
C	3.559643	-2.609392	-0.770809
C	-0.312098	3.730971	0.184824
C	-1.487286	3.029538	0.056359
C	-1.339689	-2.677641	-0.485285
C	-0.044082	-3.330975	-0.572523
C	-2.536863	-3.385970	-0.802636
C	-3.758869	-2.755378	-0.787767
C	-3.930655	2.913208	-0.052701
C	-2.788847	3.646672	0.065115
O	1.830095	1.156831	1.499761
O	2.427096	-0.616958	-1.712598
O	-0.572101	1.139777	-1.301509
O	-0.576134	-0.577643	1.884274
N	1.681341	-1.581717	1.768421
H	4.306192	3.722454	-0.291488
H	2.172066	4.869726	0.056883
H	5.639271	1.596721	-0.698515
H	5.668225	-0.815538	-1.090293
H	4.513666	-3.089643	-0.972898
H	2.467683	-4.422361	-0.689042
H	-0.028927	-4.348778	-0.962049
H	-0.350191	4.818540	0.229113
H	2.647389	-1.919064	1.756948
H	1.593266	-0.677714	2.256424
H	1.062385	-2.255936	2.286329
H	-2.473065	-4.446171	-1.038436
H	-4.669092	-3.315017	-0.990330
H	-6.002707	-1.200350	-0.724736
H	-6.076119	1.236880	-0.349914
H	-4.895426	3.415772	-0.048099
H	-2.843430	4.727640	0.173840
H	-0.721994	-1.985046	2.617687
O	-0.404524	-2.881482	3.001643
H	-0.600445	-2.869602	3.950016

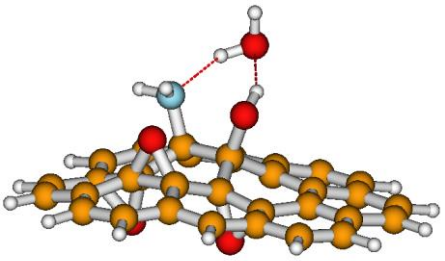


$TS_{2\text{-}3}$-H_2O

Energy=-1661.588695

C	-5.128645	0.675500	-0.334644
C	-3.931615	1.434368	-0.171650
C	-2.712074	0.762709	-0.149747
C	-2.642615	-0.653930	-0.259171
C	-3.841420	-1.387757	-0.516443
C	-5.080210	-0.685363	-0.529865
C	-1.453582	1.541350	-0.180191
C	-0.177348	0.828175	0.036439
C	-0.255144	-0.614798	0.554896
C	-1.401635	-1.343216	-0.143567
C	1.182823	-1.353068	0.372085
C	2.245094	-0.472366	-0.305463
C	2.340097	0.951313	0.158596
C	1.023800	1.643323	0.392007
C	3.494041	-1.122422	-0.810266
C	4.730646	-0.306244	-0.837244
C	4.709377	1.032034	-0.611177
C	3.517724	1.749249	-0.215364
C	0.963127	3.108645	0.206603
C	2.160486	3.786769	0.074000
C	3.406144	3.120891	-0.134464
C	1.147477	-2.726339	-0.278827
C	2.441544	-3.337780	-0.561806
C	3.563242	-2.605190	-0.754755
C	-0.332854	3.722990	0.154124
C	-1.504402	3.014550	0.036456
C	-1.327447	-2.695038	-0.454726
C	-0.028980	-3.344118	-0.535478
C	-2.520201	-3.410573	-0.770123
C	-3.745173	-2.786080	-0.758731
C	-3.947705	2.885022	-0.064648
C	-2.809338	3.624958	0.042697
O	1.823706	1.176390	1.493912
O	2.413784	-0.624512	-1.701970
O	-0.581646	1.112729	-1.302964
O	-0.589271	-0.521871	1.900630
N	1.698688	-1.585963	1.790938
H	4.284137	3.732404	-0.332714
H	2.144854	4.872573	0.010347
H	5.625568	1.608460	-0.725797
H	5.659451	-0.806705	-1.099255
H	4.518238	-3.081399	-0.961618
H	2.480419	-4.422260	-0.64979
H	-0.008158	-4.363242	-0.920446
H	-0.376285	4.810678	0.188444
H	2.628010	-2.011371	1.757707

H	1.732907	-0.672018	2.258712
H	0.982063	-2.216340	2.371361
H	-2.450502	-4.472022	-0.997443
H	-4.652629	-3.351820	-0.956593
H	-5.997021	-1.244924	-0.701585
H	-6.084544	1.194474	-0.342098
H	-4.915069	3.382384	-0.062151
H	-2.868654	4.706618	0.141149
H	-0.640518	-1.630511	2.451060
O	-0.317865	-2.699476	2.895645
H	-0.454153	-2.704708	3.854824

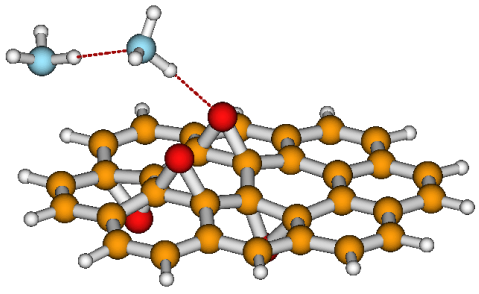


3-H_2O

Energy=-1661.617775

C	-5.111798	0.742008	-0.332570
C	-3.906420	1.487512	-0.169871
C	-2.693757	0.802699	-0.149216
C	-2.638082	-0.614228	-0.263203
C	-3.845140	-1.332345	-0.529088
C	-5.076999	-0.618028	-0.535366
C	-1.426883	1.565763	-0.184108
C	-0.153767	0.838535	0.024686
C	-0.235262	-0.612728	0.517175
C	-1.404146	-1.319398	-0.157805
C	1.186043	-1.373983	0.386527
C	2.248573	-0.480948	-0.285789
C	2.362478	0.929957	0.209517
C	1.048545	1.641111	0.405394
C	3.483240	-1.121435	-0.827274
C	4.733951	-0.325676	-0.824594
C	4.735897	1.002959	-0.551928
C	3.550711	1.723949	-0.141850
C	1.004169	3.106143	0.227521
C	2.210597	3.773720	0.131915
C	3.453517	3.096155	-0.052621
C	1.127330	-2.715355	-0.343432
C	2.411279	-3.331526	-0.663240
C	3.536276	-2.605288	-0.842992
C	-0.284294	3.734406	0.161829
C	-1.462202	3.038894	0.035672
C	-1.341177	-2.664903	-0.496960
C	-0.048619	-3.325370	-0.606592
C	-2.542090	-3.361627	-0.821658
C	-3.761508	-2.726583	-0.792756
C	-3.908037	2.938608	-0.065666
C	-2.760602	3.663942	0.039431
O	1.809719	1.159880	1.522206
O	2.410102	-0.573408	-1.695744
O	-0.559602	1.126673	-1.306690
O	-0.592031	-0.446928	1.893266
N	1.645710	-1.714774	1.766243
H	4.340914	3.699196	-0.234133
H	2.207537	4.860361	0.080439
H	5.660776	1.569335	-0.644888
H	5.655567	-0.832807	-1.099642
H	4.483464	-3.082662	-1.081724
H	2.434041	-4.411873	-0.795924
H	-0.040610	-4.331695	-1.023783
H	-0.317332	4.822323	0.202408
H	2.579223	-2.120151	1.704058
H	1.708775	-0.852812	2.307478
H	0.410207	-2.783674	2.680043
H	-2.482106	-4.418655	-1.070294
H	-4.674557	-3.281351	-0.996435
H	-5.998906	-1.167575	-0.712024
H	-6.062037	1.271121	-0.337585
H	-4.869801	3.446422	-0.064274
H	-2.806265	4.746477	0.136078
H	-0.810554	-1.323313	2.284985
O	-0.497931	-3.027450	3.002605
H	-0.451323	-3.057026	3.969845

Coordinates of Figure 13

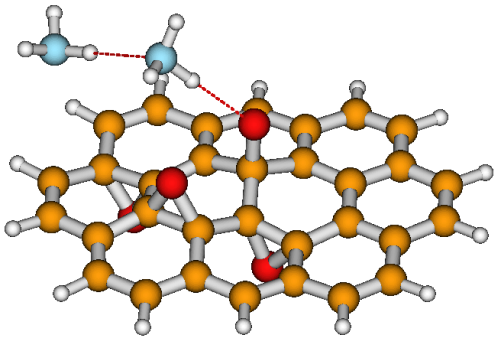


0-2NH_3

Energy= -1641.735406

C	-5.479177	-0.035558	0.355034
C	-4.385373	0.876954	0.277928
C	-3.101951	0.365552	0.090025
C	-2.868682	-1.039688	0.009522
C	-3.982473	-1.934962	0.030753
C	-5.285165	-1.391481	0.213085
C	-1.981475	1.305036	-0.142046
C	-0.598626	0.766404	-0.132961
C	-0.397312	-0.695327	0.130404
C	-1.554522	-1.578615	-0.077760
C	0.977076	-1.237615	-0.083070
C	2.014509	-0.258540	-0.551595
C	1.915077	1.171976	-0.104680
C	0.531157	1.714238	0.122347
C	3.342681	-0.779536	-0.989547
C	4.475441	0.176738	-0.970186

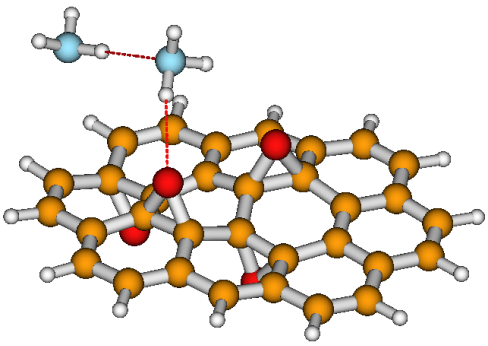
C	4.271183	1.512795	-0.846556
C	2.979282	2.096717	-0.542064
C	0.268452	3.153226	-0.098957
C	1.365730	3.958751	-0.332936
C	2.683775	3.442425	-0.549547
C	1.136483	-2.655520	-0.490373
C	2.493523	-3.099874	-0.776653
C	3.536594	-2.251172	-0.935599
C	-1.091628	3.606517	0.014912
C	-2.177187	2.763083	0.091055
C	-1.324367	-2.947331	-0.264171
C	0.025486	-3.450162	-0.479145
C	-2.457173	-3.815275	-0.295099
C	-3.734183	-3.328285	-0.127006
C	-4.571897	2.317551	0.371112
C	-3.534934	3.199354	0.293472
O	1.403729	1.409256	1.221070
O	2.278557	-0.379279	-1.944608
O	-1.238803	1.008656	-1.385733
O	0.450207	-1.047967	1.246243
N	5.516444	-1.580203	1.763086
H	3.471746	4.151595	-0.794812
H	1.219141	5.033073	-0.424066
H	5.115639	2.192770	-0.942296
H	5.475699	-0.224560	-1.095436
H	4.545721	-2.628541	-1.065141
H	2.664215	-4.173194	-0.834537
H	0.130268	-4.511351	-0.699610
H	-1.261217	4.681971	0.051188
H	5.675637	-2.534375	2.085995
H	6.301821	-1.025489	2.103146
H	4.676326	-1.237384	2.246204
H	-2.298177	-4.881685	-0.437712
H	-4.579268	-4.013098	-0.121525
H	-6.136036	-2.068530	0.240907
H	-6.482439	0.357838	0.501882
H	-5.583150	2.687992	0.521787
H	-3.721601	4.266819	0.389128
H	2.720596	-1.004470	4.165209
N	2.900271	-0.493002	3.301769
H	2.046467	-0.540209	2.743760
H	3.010143	0.487657	3.557968



$TS_{0\text{-}1}$-2NH_3

Energy= -1641.6823725

C	-5.402757	0.010533	0.321354
C	-4.312438	0.921160	0.233218
C	-3.031174	0.399001	0.046409
C	-2.814127	-1.006988	-0.027949
C	-3.926980	-1.901513	0.002090
C	-5.219919	-1.352570	0.188488
C	-1.902323	1.331238	-0.185615
C	-0.538490	0.787701	-0.184864
C	-0.328430	-0.667236	0.186512
C	-1.502284	-1.535523	-0.161892
C	0.965354	-1.190893	-0.370472
C	2.061010	-0.243773	-0.631671
C	1.967865	1.162434	-0.131175
C	0.592505	1.714195	0.105426
C	3.443406	-0.783476	-0.959333
C	4.575842	0.157352	-0.776705
C	4.377915	1.494333	-0.649159
C	3.070755	2.089097	-0.451323
C	0.361572	3.164799	-0.051812
C	1.475089	3.964375	-0.219882
C	2.795344	3.438079	-0.401437
C	1.156956	-2.548373	-0.633841
C	2.514177	-3.059641	-0.834690
C	3.596781	-2.253752	-0.897679
C	-0.998298	3.626044	0.027624
C	-2.091251	2.788770	0.054597
C	-1.297998	-2.916003	-0.407916
C	0.015151	-3.381359	-0.634011
C	-2.438301	-3.792331	-0.407364
C	-3.696511	-3.306288	-0.178621
C	-4.492169	2.363384	0.314567
C	-3.448261	3.236344	0.238505
O	1.434084	1.305785	1.194864
O	2.512197	-0.338498	-1.992814
O	-1.167318	1.027286	-1.446772
O	-0.236626	-0.892423	1.554807
N	5.108490	-1.722916	2.013588
H	3.607163	4.146252	-0.554276
H	1.346432	5.043663	-0.271744
H	5.238357	2.160529	-0.629951
H	5.577277	-0.260132	-0.789680
H	4.602190	-2.660857	-0.895840
H	2.643521	-4.139734	-0.851175
H	0.154892	-4.445721	-0.820854
H	-1.163049	4.701515	0.082373
H	5.326910	-2.666646	2.333712
H	5.768269	-1.102626	2.483423
H	4.173495	-1.494179	2.381975
H	-2.281602	-4.855353	-0.574982
H	-4.549276	-3.980150	-0.154781
H	-6.077388	-2.020303	0.225238
H	-6.404808	0.406622	0.471143
H	-5.501715	2.740690	0.458972
H	-3.628098	4.305205	0.331288
H	2.062852	-1.472882	4.087160
N	2.286374	-0.930037	3.252967
H	1.449235	-0.945612	2.655657
H	2.384527	0.038474	3.557523



1-2NH$_3$

Energy= -1641.717558

C	-5.428534	-0.010955	0.134715
C	-4.348119	0.899940	0.128465
C	-3.041109	0.379382	0.040831
C	-2.817875	-1.001592	0.023741
C	-3.900267	-1.904653	-0.020823
C	-5.210361	-1.377741	0.033847
C	-1.912409	1.331395	-0.145873
C	-0.540257	0.814685	-0.189058
C	-0.266277	-0.633955	0.078328
C	-1.440782	-1.558234	0.124844
C	1.014892	-1.139496	-0.422462
C	2.057988	-0.166785	-0.757426
C	1.956713	1.199331	-0.151613
C	0.588019	1.727693	0.143227
C	3.461510	-0.674489	-1.066128
C	4.581600	0.262632	-0.810490
C	4.371890	1.586989	-0.593414
C	3.058415	2.157103	-0.369359
C	0.341129	3.181786	0.114714
C	1.449346	3.999076	0.009226
C	2.773560	3.495581	-0.208653
C	1.209930	-2.487992	-0.612901
C	2.559235	-2.968892	-0.898972
C	3.624593	-2.141141	-1.025154
C	-1.025997	3.621582	0.199943
C	-2.114052	2.778034	0.153595
C	-1.202775	-2.972337	-0.255129
C	0.081405	-3.391881	-0.506632
C	-2.367662	-3.823307	-0.303141
C	-3.628694	-3.325976	-0.156644
C	-4.528542	2.338193	0.228149
C	-3.482210	3.213859	0.266333
O	1.424120	1.206211	1.197305
O	2.548199	-0.186066	-2.098783
O	-1.189886	1.104111	-1.428315
O	-0.737837	-1.136594	1.341665
N	5.259466	-1.822806	1.963078
H	3.582045	4.218432	-0.296267
H	1.314231	5.078389	0.037821
H	5.226607	2.256240	-0.515750
H	5.588566	-0.142547	-0.832643
H	4.633731	-2.539700	-1.061275
H	2.715240	-4.045476	-0.916692
H	0.257248	-4.446591	-0.712325
H	-1.202625	4.692105	0.297295
H	5.515139	-2.775098	2.223642
H	5.885522	-1.205134	2.479428
H	4.311915	-1.658501	2.325909
H	-2.219188	-4.888426	-0.466874
H	-4.480202	-4.001777	-0.190981
H	-6.057318	-2.059432	0.001851
H	-6.444635	0.371378	0.200603
H	-5.545837	2.714982	0.305359
H	-3.672798	4.278653	0.382018
H	2.296343	-1.160398	4.158009
N	2.320663	-1.182475	3.138929
H	1.532795	-1.758048	2.840350
H	2.099748	-0.240397	2.814975

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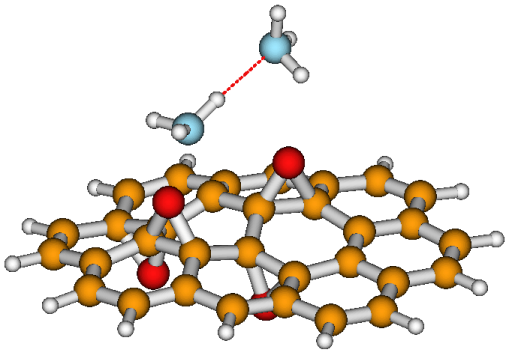
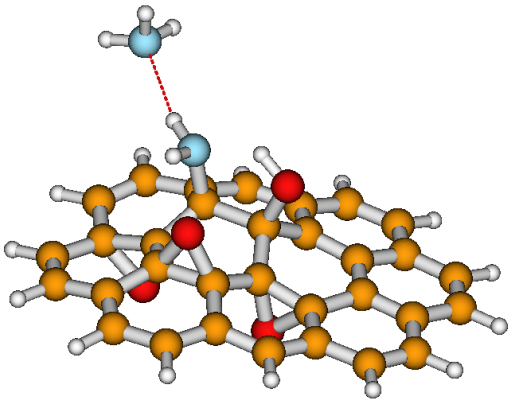


TS$_{1\text{-}2}$-2NH$_3$

Energy= -1641.6858488

C	-5.120560	0.876507	-0.330414
C	-3.912696	1.599590	-0.186156
C	-2.704966	0.873760	-0.162188
C	-2.699238	-0.522379	-0.235940
C	-3.906486	-1.240041	-0.430702
C	-5.114468	-0.500450	-0.470973
C	-1.420274	1.626758	-0.167348
C	-0.147803	0.890982	-0.012931
C	-0.171051	-0.597228	0.261145
C	-1.451572	-1.295387	-0.009473
C	1.135253	-1.326987	0.025090
C	2.275975	-0.440874	-0.402046
C	2.364018	0.927117	0.212238
C	1.065947	1.647758	0.413477
C	3.537463	-1.097239	-0.868058
C	4.796961	-0.339129	-0.673447
C	4.795210	0.977260	-0.337190
C	3.591050	1.712236	-0.011035
C	1.041819	3.121790	0.338328
C	2.263072	3.769581	0.307896
C	3.503942	3.079449	0.142286
C	1.075618	-2.626672	-0.587328
C	2.337643	-3.246311	-0.927901
C	3.522006	-2.573015	-0.973259
C	-0.240134	3.762930	0.295352
C	-1.431419	3.092501	0.127819

C	-1.408649	-2.688548	-0.485026
C	-0.170698	-3.274580	-0.732120
C	-2.664925	-3.336916	-0.703374
C	-3.859904	-2.669130	-0.625779
C	-3.875652	3.040497	-0.049995
C	-2.714603	3.739871	0.116891
O	1.768550	1.068326	1.533064
O	2.585807	-0.423350	-1.791093
O	-0.572950	1.270990	-1.326024
O	-0.912057	-1.040565	1.398912
N	1.718057	-1.681541	1.815204
H	4.408452	3.677075	0.047670
H	2.281510	4.857274	0.315840
H	5.737309	1.521516	-0.301782
H	5.732369	-0.857751	-0.867840
H	4.454996	-3.084607	-1.192988
H	2.328783	-4.313972	-1.145333
H	-0.161656	-4.293959	-1.120263
H	-0.261834	4.848684	0.379018
H	2.646980	-2.089836	1.722045
H	1.761280	-0.809044	2.342417
H	1.076385	-2.358359	2.270208
H	-2.656495	-4.396253	-0.956092
H	-4.795015	-3.198693	-0.789220
H	-6.051727	-1.033902	-0.613647
H	-6.063177	1.419534	-0.348113
H	-4.823965	3.573600	-0.061135
H	-2.743959	4.819660	0.244775
H	-0.422013	-4.415638	2.749685
N	-0.258131	-3.490588	3.144205
H	-0.994075	-2.879022	2.789343
H	-0.373708	-3.566822	4.153642



2-2NH$_3$

Energy= -1641.745427

C	-5.304202	-0.309869	-0.037715
C	-4.273411	0.668807	0.085654
C	-2.945802	0.252969	0.022232
C	-2.602808	-1.119080	-0.137141
C	-3.647151	-2.070886	-0.354868
C	-4.998976	-1.629250	-0.278903
C	-1.869066	1.265617	-0.049959
C	-0.462881	0.815297	0.076327
C	-0.214692	-0.627301	0.523263
C	-1.245737	-1.550351	-0.113820
C	1.340659	-1.071217	0.323622
C	2.141911	0.026635	-0.401137
C	1.986113	1.426792	0.116845
C	0.567212	1.844309	0.411999
C	3.439873	-0.331720	-1.039619
C	4.491191	0.710891	-1.103248
C	4.233834	2.006496	-0.794579
C	2.956356	2.456457	-0.286222
C	0.208929	3.270738	0.277957
C	1.242112	4.177329	0.130454
C	2.582824	3.776876	-0.150913
C	1.514245	-2.390571	-0.424750
C	2.870574	-2.717050	-0.856921
C	3.799755	-1.769570	-1.101831
C	-1.183619	3.617251	0.302644
C	-2.197490	2.693772	0.217714
C	-0.922761	-2.852018	-0.472699
C	0.473661	-3.224435	-0.650132
C	-1.967757	-3.781244	-0.751807
C	-3.290092	-3.414068	-0.652762
C	-4.570484	2.084982	0.236781
C	-3.595132	3.032678	0.308076
O	1.482872	1.517947	1.467046
O	2.213777	-0.015061	-1.820621
O	-0.995292	1.041633	-1.226152
O	-0.520785	-0.653527	1.914822
N	1.902328	-1.279844	1.679044
H	3.311630	4.554455	-0.371125
H	1.010456	5.240115	0.109912
H	5.010012	2.756745	-0.934846
H	5.476584	0.414063	-1.454404
H	4.802484	-2.033640	-1.429285
H	3.105689	-3.766348	-1.028849
H	0.670621	-4.194487	-1.106706
H	-1.438808	4.673499	0.378116
H	2.333630	-0.434263	2.042796
H	0.295390	-1.039495	2.331068
H	2.562705	-2.058550	1.748232
H	-1.703868	-4.800173	-1.027264
H	-4.077635	-4.144058	-0.825888
H	-5.795476	-2.356376	-0.421297
H	-6.342651	0.008442	0.021225
H	-5.615301	2.379900	0.303422
H	-3.860000	4.079187	0.442475
H	4.671127	-3.800820	2.180736
N	3.762383	-3.619266	2.604010
H	3.221172	-4.480162	2.536226
H	3.921563	-3.447800	3.596068