Supporting Information

Mechanistic study on guanidines-catalyzed chemical fixation of CO_2 with 2-aminobenzonitrile to quinazoline-2,4(1*H*,3*H*)-dione

*Weiyi Li**[a] *Na Yang*[b] *and Yajing Lyu*[a]

[a] School of Science, Xihua University, Chengdu, Sichuan, 610039, P. R. China.

[b] Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang, 621900, P. R. China

E-mail: weiyili@mail.xhu.edu.cn; Fax:+86-028-87727663; Tel: +86-028-87727663

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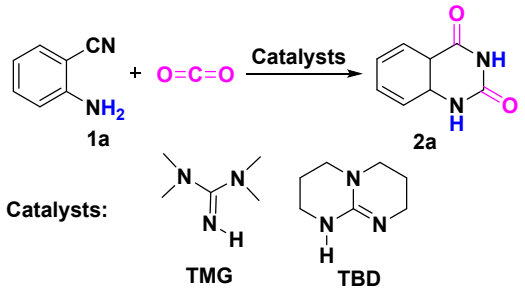
S1: Computational details.



Optimization and frequency calculation in gas phase: M06-2X/6-31G+(d)

Solvation Method: M06-2X/6–31++G(d, p)

For single-point energy calculation, the SCRF = (Generic, Read, SMD, ExternalIteration, DoVacuum) keyword was used.

Solvent parameter:

eps=7.01/25.57

RSolv=4.01

S2: Mechanism of TBD-catalyzed chemical fixation of CO_2 with 1a

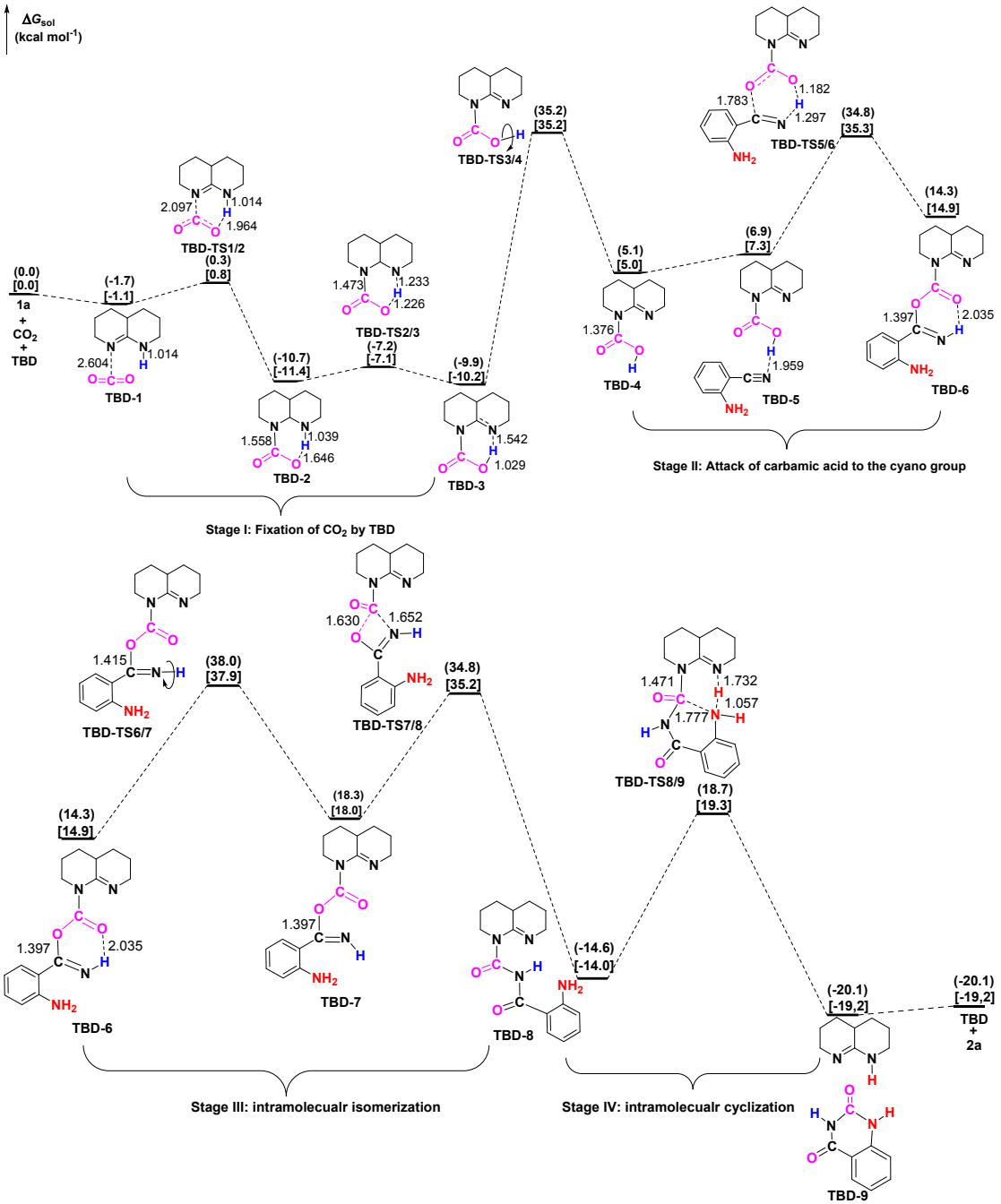
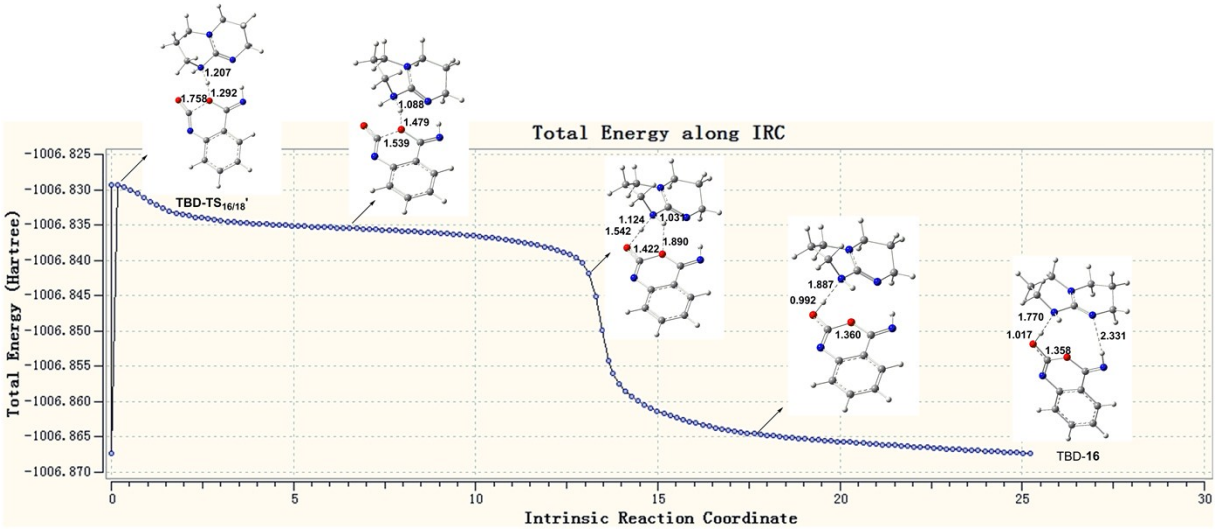


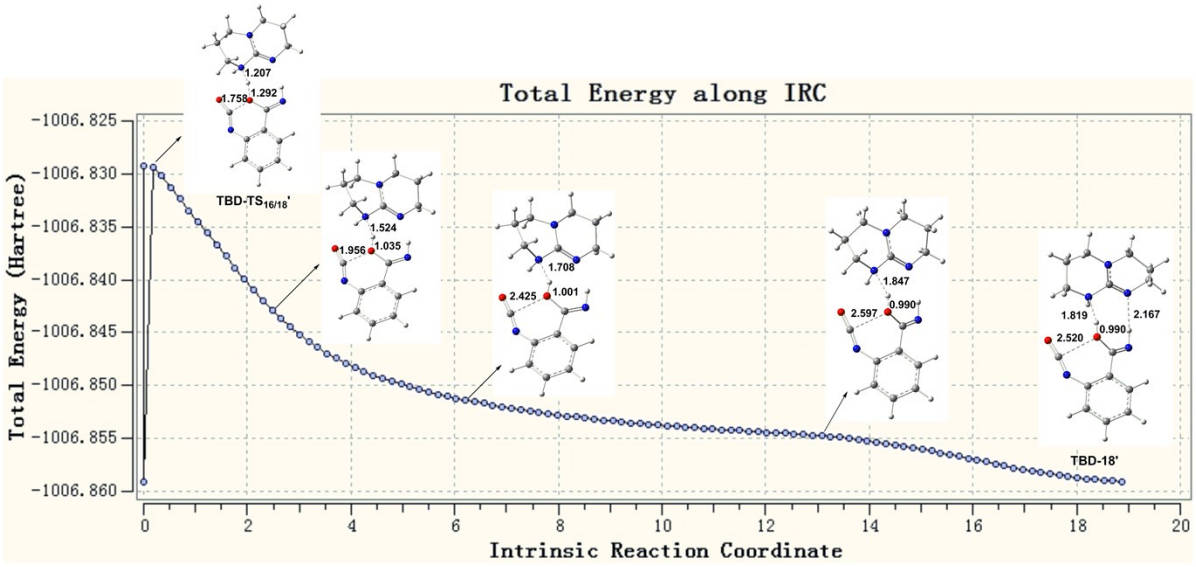
Fig. S1 The covalent bonding mechanism for TMG-catalyzed reaction of CO_2 with **1a**. The ΔG_{sol} in the solvents with the dielectric constants of 7.01 and 25.57 are given in parentheses and square brackets, respectively. The bond lengths of the optimized-structures are labelled in Å.

From TBD-**$TS_{16/18}$'** to TBD-**16**:



(a)

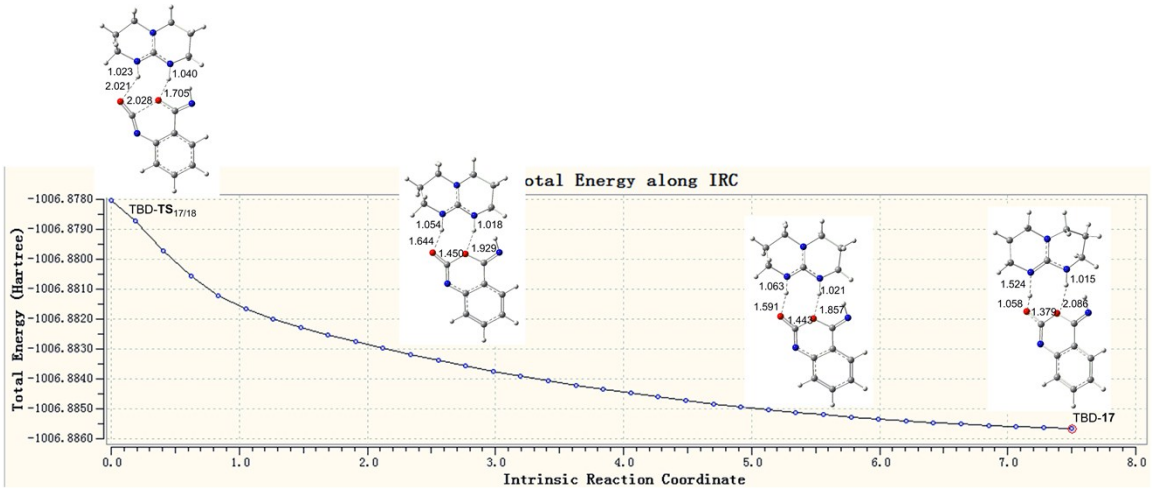
From TBD-**$TS_{16/18}$'** to TBD-**18'**:



(b)

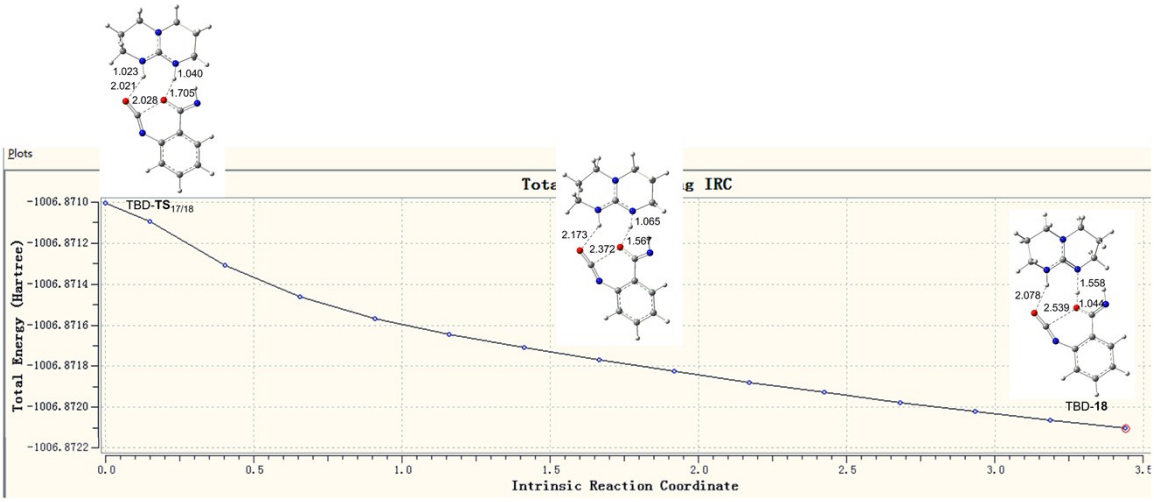
Figure S2. IRC scan of the ring-opening transtion state TBD-**$TS_{16/18}$'**

From TBD-**$TS_{17/18}$** to TBD-**17**:



(a)

From TBD-**$TS_{17/18}$** to TBD-**18**:



(b)

Figure S2. IRC scan of the ring-opening transtion state TBD-**$TS_{17/18}$**

S3 Energy summary

Table S1 Electronic chemical potential μ, chemical hardness η, global electrophilicity ω, and global nucleophilicity N for reactants, catalysts and key intermediates.

	HOMO (hartree)	LUMO (hartree)	μ (hartree)	η (hartree)	ω (eV)	N (eV)
1a	-0.27947	-0.02029	-0.29976	0.25918	4.7	3.2
CO_2	-0.45117	-0.00186	-0.45303	0.44931	6.2	-1.5
TMG	-0.28086	-0.00574	-0.28660	0.27512	4.1	3.2
TBD	-0.25944	-0.00493	-0.26437	0.25451	3.7	3.7
TMG-**14**	-0.26374	-0.01084	-0.27458	0.25290	4.1	3.6
TMG-**19**	-0.23563	-0.02482	-0.26045	0.21081	4.4	4.4
TDB-**13**	-0.26383	-0.01660	-0.28043	0.24723	4.3	3.6
TBD-**16**	-0.26497	-0.01496	-0.27993	0.25001	4.3	3.6

Table S2 Energies of the species involved in the uncatalyzed chemical fixation of CO_2 with **1a**.

	$^{a}H_c$	$^{b}G_c$	$^{c}E_{sol,anilinec}$	$^{d}\Delta H_{sol,aniline}^{\neq}$	$^{e}\Delta G_{sol,aniline}^{\neq}$	$E_{sol,benzonitrile}$	$\Delta H_{sol,benzonitrile}^{\neq}$	$\Delta G_{sol,benzonitrile}^{\neq}$
CO_2	0.01549	-0.00942	-188.51785	-	-	-188.51825	-	-
1a	0.12544	0.08524	-379.72897	-	-	-379.73191	-	-
b-**1**	0.14245	0.09045	-568.25199	-2.3	1.6	-568.25503	-2.1	1.8
b-**TS$_{1/2}$**	0.13841	0.09076	-568.18107	39.7	46.3	-568.18481	39.4	46.1
b-**TS$_{1/2}$'**	0.26888	0.20350	-947.95573	14.2	30.6	-947.96303	13.5	30.0
b-**2**	0.14328	0.09456	-568.24480	2.7	8.7	-568.24855	2.5	8.5
b-**TS$_{2/3}$**	0.14205	0.09530	-568.24095	4.4	11.6	-568.24525	3.8	11.0
b-**3**	0.14313	0.09504	-568.24113	5.0	11.3	-568.24551	4.3	10.7
b-**TS$_{3/4}$**	0.13790	0.09231	-568.17586	42.6	50.6	-568.17998	42.1	50.1
b-**TS$_{3/4}$'**	0.26691	0.20097	-947.94906	17.1	33.2	-947.95454	17.6	33.7
b-**4**	0.14433	0.09996	-568.25864	-5.3	3.4	-568.26197	-5.3	3.4
b-**TS$_{4/5}$**	0.13876	0.09516	-568.17645	42.8	52.0	-568.17860	43.6	52.7
b-TS$_{4/5}$'	0.26840	0.20384	-947.96696	6.8	23.8	-947.97231	7.4	24.4
b-**5**	0.14421	0.10059	-568.23696	8.2	17.4	-568.23935	8.8	18.0
b-**TS$_{5/6}$**	0.14240	0.09907	-568.22529	14.4	23.8	-568.22817	14.7	24.1
b-**6**	0.14398	0.10023	-568.23414	9.9	19.0	-568.23703	10.2	19.3

b-**TS$_{6/7}$**	0.13744	0.09377	-568.15184	57.4	66.6	-568.15439	57.9	67.1
b-**TS$_{6/7}$'**	0.26745	0.20060	-947.94356	20.9	36.4	-947.95038	20.6	36.1
b-**7**	0.14313	0.09577	-568.22397	15.7	22.5	-568.22681	16.0	22.9
b-**TS$_{7/8}$**	0.14209	0.09652	-568.21985	17.7	25.6	-568.22304	17.8	25.7
b-**8**	0.14341	0.09565	-568.22566	14.8	21.4	-568.22819	15.4	21.9
b-**TS$_{8/9}$**	0.14165	0.09697	-568.22427	14.6	23.1	-568.22750	14.7	23.2
b-**9**	0.14365	0.09990	-568.24876	0.5	9.6	-568.25415	-0.8	8.3
b-**TS$_{9/10}$**	0.13875	0.09561	-568.19836	29.0	38.5	-568.20197	28.9	38.4
b-**TS$_{9/10}$'**	0.26545	0.20256	-947.97509	-0.1	17.9	-947.98064	0.3	18.3
b-**10**	0.14472	0.10175	-568.26532	-9.2	0.4	-568.26795	-8.8	0.8
b-**TS$_{10/11}$**	0.14294	0.10024	-568.25371	-3.1	6.7	-568.25653	-2.7	7.0
b-**11**	0.14483	0.10191	-568.26654	-9.9	-0.3	-568.26884	-9.3	0.3
b-**TS$_{11/12}$**	0.13939	0.09652	-568.20538	25.0	34.7	-568.20739	25.9	35.5
b-**TS$_{11/12}$'**	0.26866	0.20495	-947.99008	-7.5	10.0	-947.99483	-6.6	10.9
b-**12**	0.14489	0.10167	-568.27665	-16.2	-6.8	-568.27924	-15.8	-6.3
b-**TS$_{12/13}$**	0.13951	0.09634	-568.21843	16.9	26.4	-568.22085	17.5	27.0
b-**TS$_{12/13}$'**	0.26877	0.20469	-948.00336	-15.8	1.5	-948.00832	-15.0	2.3
b-**13**	0.14515	0.10143	-568.29584	-28.1	-19.0	-568.29910	-28.1	-18.9

a: H_C is the enthalpy correction calculated at the M06-2X/6-31+G(d)] level in gas phase;

b: G_C is the Gibbs free energy correction calculated at the M06-2X/6-31+G(d)] level in gas phase;

c: E_{sol} is the electron energy in solvent after PCM correction calculated at the M06-2X/(SMD, aniline)//6-311++G(d, p) level;

d: $\Delta H_{sol,\ \text{aniline}}^{\neq}$ is the relative enthalpy energy, $H_{sol,\ \text{aniline}} = H_c + H_{sol}$, The sum of H_{sol} (CO_2) + H_{sol} (1a) is set as zero energy reference;

e: $\Delta G_{sol\ \text{aniline}}^{\neq}$ is the relative Gibbs free energy, $G_{sol\ \text{aniline}} = G_c + G_{sol,\text{aniline}}$ (CO_2) + $G_{sol,\ \text{aniline}}$ (1a) is set as zero energy reference; $\Delta G_{sol\ \text{aniline}}^{\neq} = [G_{sol\ \text{aniline}} - G_{sol,\text{aniline}}\ (CO_2) - G_{sol,\ \text{aniline}}\ (1a)] + (n - m) \times 4.3$, n and m are components.

Table S3 Energies of the species involved in TMG-catalyzed chemical fixation of CO_2 with **1a**.

	H_c	G_c	$E_{sol,anilinec}$	$\Delta H_{sol,aniline}^{\neq}$	$\Delta G_{sol,aniline}^{\neq}$	$E_{sol,benzonitrile}$	$\Delta H_{sol,benzonitrile}^{\neq}$	$\Delta G_{sol,benzonitrile}^{\neq}$
TMG	0.20190	0.15671	-362.45615			-362.4585	-1309.972	
TMG-**1**	0.21892	0.16169	-550.98043	-3.1	0.7	-550.9825	-2.7	1.1
TMG-**TS$_{1/2}$**	0.21839	0.16591	-550.97792	-1.8	4.9	-550.9779	-0.1	6.7
TMG-**2**	0.21976	0.16703	-550.98470	-5.2	1.4	-550.989	-6.2	0.4
TMG-**TS$_{2/3}$**	0.21508	0.16307	-550.93597	22.4	29.5	-550.936	24.1	31.2
TMG-**3**	0.22033	0.16888	-550.98582	-5.6	1.8	-550.9887	-5.7	1.7
TMG-**TS$_{3/4}$**	0.21832	0.16714	-550.97015	3.0	10.6	-550.9737	2.5	10.1
TMG-**TS$_{3/4}$'**	0.34346	0.27201	-930.70702	-2.1	13.6	-930.7123	-1.9	13.9
TMG-**4**	0.22037	0.16854	-550.98633	-5.9	1.3	-550.9893	-6.0	1.2
TMG-**5**	0.34805	0.27215	-930.72243	-8.9	4.0	-930.7274	-8.5	4.5
TMG-**TS$_{5/6}$**	0.34295	0.27175	-930.68454	11.6	27.6	-930.6894	12.2	28.1
TMG-**TS$_{5/6}$'**	0.47012	0.38313	-1310.40798	16.2	43.1	-1310.41492	17.3	44.2
TMG-**6**	0.34917	0.27968	-930.72159	-7.7	9.3	-930.7262	-7.0	10.0
TMG-**TS$_{2/6}$'**	0.34326	0.27320	-930.68268	13.0	29.6	-930.6827	16.6	33.2
TMG-**6'**	0.34895	0.27770	-930.71532	-3.9	12.0	-930.7198	-3.2	12.7
TMG-**TS$_{6/7}$**	0.34559	0.27353	-930.67544	19.0	34.4	-930.6807	19.3	34.7
TMG-**7**	0.34865	0.27758	-930.71415	-3.4	12.6	-930.7196	-3.2	12.8
TMG-**TS$_{7/8}$**	0.34627	0.27659	-930.66711	24.7	41.5	-930.6721	25.1	42.0
TMG-**8**	0.34936	0.27812	-930.74115	-19.9	-4.0	-930.7461	-19.4	-3.5
TMG-**TS$_{8/9}$**	0.34789	0.27794	-930.73508	-17.0	-0.3	-930.7401	-16.6	0.1
TMG-**9**	0.34982	0.27834	-930.73593	-16.3	-0.5	-930.7409	-15.8	-0.1
TMG-**TS$_{9/10}$**	0.34657	0.27787	-930.66044	29.0	46.5	-930.6662	29.0	46.5
TMG-**TS$_{9/10}$'**	0.46989	0.38199	-1310.42338	6.4	32.8	-1310.42948	8.0	34.4
TMG-**10**	0.34917	0.28138	-930.72330	-8.8	9.3	-930.7279	-8.1	10.0
TMG-**TS$_{10/11}$**	0.34769	0.27925	-930.71602	-5.1	12.5	-930.7215	-5.0	12.7
TMG-**11**	0.34890	0.28098	-930.72267	-8.5	9.4	-930.7282	-8.5	9.5
TMG-**TS$_{11/12}$**	0.34416	0.27644	-930.68493	12.2	30.3	-930.6897	12.7	30.9
TMG-**TS$_{11/12}$'**	0.47360	0.38676	-1310.45098	-8.6	22.7	-1310.45815	-7.7	23.7
TMG-**12**	0.34933	0.27868	-930.76140	-32.6	-16.3	-930.7663	-32.1	-15.8
TMG-**13**	0.34693	0.26620	-930.71950	-7.8	2.2	-930.7231	-6.469515	3.5
TMG-**TS$_{13/14}$**	0.34305	0.26908	-930.70389	-0.4	13.8	-930.7092	-0.177145	14.0

TMG-**14**	0.34736	0.27162	-930.72861	-13.2	-0.2	-930.7336	-12.77613	0.3
TMG-**TS$_{14/15}$**	0.34439	0.27441	-930.69586	5.4	22.1	-930.7006	6.0143591	22.7
TMG-**15**	0.34876	0.27491	-930.72143	-7.9	6.4	-930.7259	-7.072366	7.2
TMG-**TS$_{15/16}$**	0.34360	0.27287	-930.64109	39.3	55.5	-930.6446	40.710557	56.9
TMG-**TS$_{15/16}$'**	0.47220	0.37796	-1310.42864	4.5	26.9	-1310.435	5.8716129	28.3
TMG-**16**	0.34856	0.27489	-930.69990	5.5	19.9	-930.7037	6.7280324	21.1
TMG-**TS$_{16/17}$**	0.34693	0.27648	-930.68916	11.2	27.6	-930.6936	12.003963	28.4
TMG-**17**	0.34815	0.27349	-930.69708	7.0	20.8	-930.7015	7.8419616	21.6
TMG-**TS$_{17/18}$**	0.34715	0.27325	-930.69622	6.9	21.2	-930.7001	8.114114	22.3
TMG-**18**	0.34748	0.27524	-930.72251	-9.3	5.9	-930.7285	-9.498033	5.8
TMG-**TS$_{18/19}$**	0.34390	0.27271	-930.71716	-8.2	7.7	-930.7217	-7.514437	8.4
TMG-**19**	0.34847	0.28084	-930.73331	-15.5	2.7	-930.7398	-15.9819	2.2
TMG-**TS$_{19/20}$**	0.34535	0.27182	-930.70502	0.3	14.8	-930.7112	-0.011899	14.5
TMG-**20**	0.34715	0.27319	-930.72015	-8.1	6.1	-930.7252	-7.662379	6.5
TMG-**TS$_{20/21}$**	0.34655	0.27348	-930.69916	4.7	19.5	-930.7029	5.9512621	20.7
TMG-**21**	0.34801	0.27383	-930.70491	2.0	16.1	-930.7082	3.551202	17.6
TMG-**TS$_{21/22}$**	0.34649	0.27429	-930.70485	1.1	16.4	-930.7083	2.5314925	17.8
TMG-**22**	0.34394	0.27284	-930.74654	-26.6	-10.7	-930.7535	-27.46054	-11.5
TMG-**TS$_{22/23}$**	0.34782	0.27590	-930.74032	-20.3	-4.8	-930.7459	-20.2483	-4.8
TMG-**23**	0.34901	0.28065	-930.76682	-36.2	-18.5	-930.7718	-35.71058	-18.0
TMG-**TS$_{23/24}$**	0.34395	0.27545	-930.75001	-28.8	-11.2	-930.7549	-28.32213	-10.7
TMG-**24**	0.34876	0.27858	-930.75450	-28.6	-12.0	-930.7587	-27.67262	-11.1
TMG-**TS$_{24/25}$**	0.34684	0.27578	-930.73511	-17.7	-1.6	-930.7391	-16.60537	-0.6
TMG-**25**	0.34858	0.27649	-930.74754	-24.4	-9.0	-930.7509	-22.8971	-7.5
TMG-**TS$_{25/26}$**	0.34307	0.27004	-930.69003	8.3	23.1	-930.69313	9.9	24.1
TMG-**TS$_{25/26}$'**	0.47006	0.38106	-1310.46975	-22.6	7.4	-1310.476	-20.88032	9.1
TMG-**26**	0.34883	0.27605	-930.76406	-34.6	-19.6	-930.7683	-33.65464	-18.7

Table S4 Energies of the species involved in TBD-catalyzed chemical fixation of CO_2 with **1a**.

	H_c	G_c	$E_{sol,anilinec}$	$\Delta H_{sol,aniline}^{\neq}$	$\Delta G_{sol,aniline}^{\neq}$	$E_{sol,benzonitrile}$	$\Delta H_{sol,benzonitrile}^{\neq}$	$\Delta G_{sol,benzonitrile}^{\neq}$
TBD	0.21848	0.17491	-438.66429			-438.66690		
TBD-**1**	0.23517	0.18081	-627.19338	-6.3	-1.7	-627.19541	-5.7	-1.1
TBD-**TS$_{1/2}$**	0.23427	0.18287	-627.19224	-6.2	0.3	-627.19436	-5.6	0.8
TBD-**2**	0.23568	0.18571	-627.21259	-18.0	-10.7	-627.21669	-18.7	-11.4
TBD-**TS$_{2/3}$**	0.23136	0.18257	-627.20812	-17.9	-9.9	-627.21157	-18.2	-10.2
TBD-**3**	0.23528	0.18551	-627.20676	-14.6	-7.2	-627.20958	-14.5	-7.1
TBD-**TS$_{3/4}$**	0.23222	0.18167	-627.14221	24.0	30.9	-627.14520	24.0	30.9
TBD-**4**	0.23602	0.18542	-627.18703	-1.8	5.1	-627.19021	-1.9	5.0
TBD-**5**	0.35866	0.29009	-1006.89224	11.4	32.2	-1006.89744	11.8	32.7
TBD-**TS$_{5/6}$**	0.36358	0.28793	-1006.92358	-5.2	6.9	-1006.92894	-4.8	7.3
TBD-**6**	0.35742	0.29003	-1006.88129	17.5	34.8	-1006.88639	18.0	35.3
TBD-**TS$_{6/7}$**	0.36462	0.29491	-1006.91871	-1.5	14.3	-1006.92376	-0.9	14.9
TBD-**7**	0.36168	0.29097	-1006.87706	22.8	38.0	-1006.88318	22.7	37.9
TBD-**TS$_{7/8}$**	0.36459	0.29423	-1006.91167	2.9	18.3	-1006.91815	2.6	18.0
TBD-**8**	0.37457	0.27778	-1006.86892	36.0	34.8	-1006.87432	36.3	35.2
TBD-**TS$_{8/9}$**	0.37762	0.27693	-1006.94692	-11.1	-14.6	-1006.95193	-10.5	-14.0
TBD-**9**	0.36321	0.29783	-1006.91466	0.2	18.7	-1006.91969	0.7	19.3
TBD -**10**	0.36298	0.28493	-1006.93341	-11.8	-1.2	-1006.93706	-10.3	0.3
TBD-**TS$_{10/11}$**	0.35965	0.28711	-1006.92201	-6.7	7.4	-1006.92682	-6.0	8.1
TBD-**11**	0.36379	0.29458	-1006.95830	-26.9	-10.7	-1006.96329	-26.3	-10.1
TBD-**TS$_{11/12}$**	0.36393	0.29480	-1006.95425	0.6	-8.0	-1006.95918	-23.6	-7.4
TBD-**12**	0.36409	0.29089	-1006.96443	-30.0	-16.9	-1006.96925	-29.8	-16.2
TBD-**TS$_{12/13}$**	0.36220	0.29122	-1006.95565	-26.2	-11.2	-1006.96132	-27.9	-11.0
TBD-**13**	0.36396	0.29302	-1006.96066	-28.2	-13.2	-1006.96604	-27.9	-12.8
TBD-**TS$_{13/14}$**	0.35917	0.28921	-1006.92486	-8.8	6.9	-1006.92988	-8.2	7.5
TBD-**14**	0.36500	0.29399	-1006.93710	-12.8	2.2	-1006.94195	-12.1	2.9

TBD-**TS$_{14/15}$**	0.35926	0.28839	-1006.85408	35.7	50.8	-1006.85765	37.2	52.3
TBD-**TS$_{14/15}$'**	0.48823	0.39643	-1386.64460	-0.7	22.2	-1386.65170	0.4	23.3
TBD-**15**	0.36474	0.29410	-1006.91433	1.3	16.6	-1006.91842	2.5	17.8
TBD-**TS$_{15/16}$**	0.36250	0.29172	-1006.90289	7.1	22.3	-1006.90729	8.1	23.2
TBD-**16**	0.36493	0.29576	-1006.92321	-4.1	12.0	-1006.92758	-3.1	13.1
TBD-**TS$_{16/18}$'**	0.35974	0.29114	-1006.88826	14.5	31.1	-1006.89426	14.5	31.1
TBD-**18'**	0.36407	0.29170	-1006.91031	3.4	17.6	-1006.91443	4.6	18.8
TBD-**TS$_{16/17}$**	0.36338	0.29611	-1006.91541	-0.2	17.2	-1006.91973	0.8	18.2
TBD-**17**	0.36330	0.29303	-1006.92940	-9.0	6.5	-1006.93367	-8.0	7.5
TBD-**TS$_{17/18}$**	0.36301	0.29189	-1006.92664	-7.5	11.8	-1006.93207	-7.2	12.1
TBD-**18**	0.36269	0.28817	-1006.92104	-4.2	8.6	-1006.92474	-2.8	10.1
TBD-**TS$_{18/19}$**	0.36224	0.29043	-1006.91578	-1.2	13.4	-1006.91965	0.2	14.7
TBD-**19**	0.36324	0.28837	-1006.91912	-2.6	10.0	-1006.92261	-1.1	11.5
TBD-**TS$_{19/20}$**	0.36213	0.28976	-1006.91902	-3.3	10.9	-1006.92258	-1.8	12.4
TBD-**20**	0.36461	0.29690	-1006.97618	-37.6	-20.5	-1006.98395	-38.7	-21.6
TBD-**TS$_{20/21}$**	0.36515	0.30007	-1006.97709	-37.8	-19.1	-1006.98384	-38.3	-19.6
TBD-**21**	0.36457	0.29597	-1006.99073	-46.7	-30.2	-1006.99567	-46.1	-29.5
TBD-**TS$_{21/22}$**	0.36472	0.29459	-1006.98272	-41.6	-26.0	-1006.98642	-40.2	-24.6
TBD-**22**	0.36028	0.29291	-1006.98359	-44.9	-27.6	-1006.98772	-43.8	-26.5

S4: Cartesian coordinates and 3D structures of the reactants, products, intermediates and transition states involved in the reaction

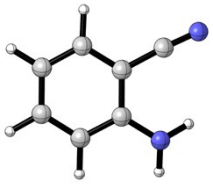
4.1 Background reaction

CO_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.162785
3	8	0	0.000000	0.000000	-1.162785

1a



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.006560	0.905458	-0.007122
2	6	0	-1.393717	1.127626	0.003285
3	6	0	-2.280839	0.062557	0.009995
4	6	0	-1.824995	-1.260607	0.004027
5	6	0	0.446151	-0.431377	-0.010287
6	6	0	-0.459994	-1.499888	-0.005444
7	6	0	1.860432	-0.667493	-0.002393
8	7	0	3.012872	-0.792088	0.014672
9	1	0	-2.526595	-2.087423	0.008344
10	1	0	-3.347963	0.265451	0.018556
11	1	0	-1.763890	2.149396	-0.001663
12	1	0	-0.070605	-2.513303	-0.006393
13	7	0	0.882495	1.955331	-0.068631
14	1	0	1.849097	1.767249	0.167942
15	1	0	0.549514	2.858273	0.238568

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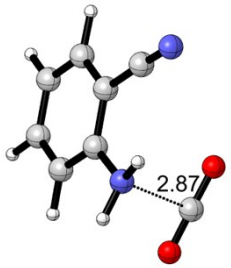
b-**1**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.084476	-1.463957	0.861110
2	6	0	-0.162532	-0.083596	0.812547
3	6	0	-1.240185	0.370574	0.024687
4	6	0	-2.039318	-0.530934	-0.688101
5	6	0	-1.782230	-1.892487	-0.628456
6	6	0	-0.716236	-2.349169	0.152481
7	1	0	0.919607	-1.829940	1.452758
8	1	0	-2.858884	-0.143342	-1.285263
9	1	0	-2.400428	-2.590693	-1.181997
10	1	0	-0.503454	-3.412888	0.207948
11	6	0	-1.496983	1.781097	-0.023511
12	7	0	-1.661269	2.928296	-0.009982
13	7	0	0.681541	0.812781	1.445980
14	1	0	0.321855	1.749228	1.594306
15	1	0	1.201594	0.453804	2.236353
16	6	0	2.461560	0.213403	-0.726220
17	8	0	1.824098	0.821920	-1.483139
18	8	0	3.116713	-0.407331	0.010225

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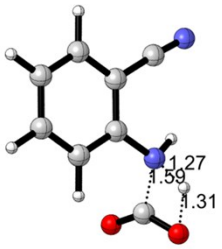
b-**TS$_{1/2}$**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.085293	-1.492974	-0.187738
2	6	0	0.107773	-0.101559	-0.136302
3	6	0	1.334843	0.566429	0.000301
4	6	0	2.529083	-0.157737	0.075007
5	6	0	2.499334	-1.545111	0.015158

6	6	0	1.277886	-2.206377	-0.114791
7	1	0	-0.863586	-2.014926	-0.270193
8	1	0	3.466476	0.378332	0.181592
9	1	0	3.424101	-2.109122	0.074600
10	1	0	1.249120	-3.290741	-0.153098
11	6	0	1.337382	2.002133	0.065281
12	7	0	1.272605	3.157234	0.119350
13	7	0	-1.104846	0.637615	-0.254015
14	1	0	-1.027009	1.585133	0.126584
15	1	0	-1.911567	0.571507	-1.233045
16	6	0	-2.463673	-0.060838	0.189855
17	8	0	-2.647387	-0.522269	1.271727
18	8	0	-3.072534	0.058779	-0.924778

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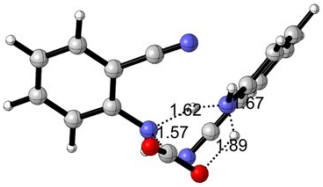
b-**TS$_{1/2}$'**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.350040	-0.281032	0.484683
2	1	0	1.266104	-0.925676	1.669999
3	6	0	-3.021136	-0.940611	-1.283313
4	6	0	-2.160963	-0.299301	-0.391548
5	6	0	-2.368493	1.067962	-0.131176
6	6	0	-3.423272	1.766860	-0.724890
7	6	0	-4.273373	1.109586	-1.604904
8	6	0	-4.060844	-0.240910	-1.887735
9	1	0	-2.877399	-1.998253	-1.487120
10	1	0	-3.560731	2.819074	-0.496711
11	1	0	-5.093830	1.645174	-2.070736
12	1	0	-4.721277	-0.759384	-2.576682
13	6	0	-1.413027	1.741435	0.703416
14	7	0	-0.565783	2.241995	1.316860
15	7	0	-1.103613	-0.964513	0.257964
16	1	0	-0.886172	-1.863604	-0.173532
17	6	0	-1.269231	-1.217446	1.802170
18	8	0	-2.255551	-0.713835	2.302307
19	8	0	-0.282602	-1.851973	2.223400

20	7	0	1.259511	-0.060332	1.086191
21	6	0	2.456589	0.249198	0.345039
22	6	0	2.866963	-0.609841	-0.681927
23	6	0	3.180023	1.396912	0.634323
24	6	0	4.028227	-0.320114	-1.404551
25	6	0	4.760820	0.823877	-1.105589
26	6	0	4.334207	1.681477	-0.093210
27	6	0	2.069862	-1.765494	-0.995595
28	7	0	1.392652	-2.672902	-1.235616
29	1	0	2.837028	2.066482	1.418213
30	1	0	4.339919	-0.992570	-2.196938
31	1	0	5.660883	1.048654	-1.667921
32	1	0	4.899443	2.579328	0.134682
33	1	0	0.973731	0.716999	1.695565

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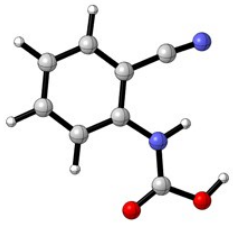
b-**2**

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.448830	-1.564748	0.000363
2	6	0	0.162825	-0.195010	0.000285
3	6	0	1.239799	0.718836	-0.000079
4	6	0	2.565032	0.274304	-0.000339
5	6	0	2.837020	-1.086055	-0.000282
6	6	0	1.774253	-1.989474	0.000065
7	1	0	-0.361629	-2.279603	0.000637
8	1	0	3.364800	1.007959	-0.000605
9	1	0	3.862768	-1.438308	-0.000496
10	1	0	1.974793	-3.056686	0.000127
11	6	0	0.944829	2.123444	-0.000127
12	7	0	0.614643	3.234718	-0.000114
13	7	0	-1.133233	0.338072	0.000624
14	1	0	-1.177805	1.350762	0.000972
15	1	0	-3.242792	1.349624	-0.000035
16	6	0	-2.319682	-0.373761	0.000069
17	8	0	-2.409574	-1.572429	-0.000439

18	8	0	-3.428858	0.398868	-0.000049

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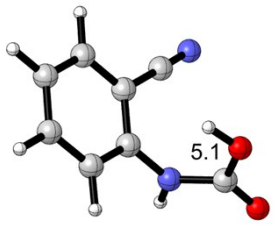
b-$TS_{2/3}$



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.096385	-1.568378	-0.377221
2	6	0	-0.273643	-0.443360	-0.418625
3	6	0	-0.818300	0.815095	-0.102055
4	6	0	-2.166160	0.933672	0.252836
5	6	0	-2.974006	-0.198688	0.285682
6	6	0	-2.441341	-1.447155	-0.031985
7	1	0	-0.662497	-2.534228	-0.618370
8	1	0	-2.567516	1.912689	0.494204
9	1	0	-4.020149	-0.104942	0.559000
10	1	0	-3.071570	-2.330620	-0.007047
11	6	0	0.014847	1.988594	-0.155400
12	7	0	0.668001	2.942890	-0.192440
13	7	0	1.094851	-0.570391	-0.772981
14	1	0	1.363588	-0.540107	-1.749044
15	1	0	0.888473	-0.528444	1.561430
16	6	0	2.167513	-0.578768	0.104113
17	8	0	3.309515	-0.624657	-0.267990
18	8	0	1.847304	-0.561333	1.414703

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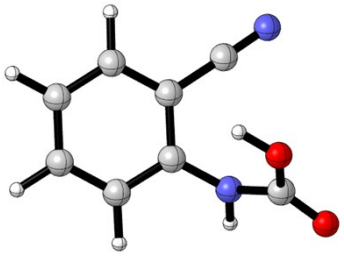
b-**3**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204846	-1.597136	-0.251944
2	6	0	-0.306761	-0.532098	-0.347778
3	6	0	-0.778138	0.776946	-0.132521
4	6	0	-2.118281	0.998358	0.211195

5	6	0	-2.998255	-0.072329	0.301637
6	6	0	-2.542093	-1.368366	0.056813
7	1	0	-0.836022	-2.606110	-0.412173
8	1	0	-2.456878	2.015257	0.382090
9	1	0	-4.038047	0.103837	0.556802
10	1	0	-3.227382	-2.207703	0.124265
11	6	0	0.105744	1.900938	-0.300629
12	7	0	0.798639	2.819283	-0.426069
13	7	0	1.045007	-0.761514	-0.682067
14	1	0	1.245828	-1.349222	-1.482050
15	1	0	0.996898	0.171694	1.495165
16	6	0	2.157651	-0.585143	0.136329
17	8	0	3.257084	-0.927163	-0.208387
18	8	0	1.932912	-0.030231	1.340167

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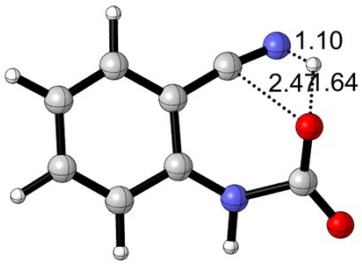
b-$\mathbf{TS_{3/4}}$



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.484674	-1.549300	-0.164195
2	6	0	-0.393610	-0.636483	-0.194553
3	6	0	-0.739081	0.749192	-0.089800
4	6	0	-2.066259	1.177718	0.186314
5	6	0	-3.075441	0.255583	0.252215
6	6	0	-2.769278	-1.113227	0.049284
7	1	0	-1.274967	-2.609119	-0.277262
8	1	0	-2.258556	2.239224	0.306151
9	1	0	-4.096072	0.565260	0.445528
10	1	0	-3.571232	-1.845221	0.085771
11	6	0	0.284012	1.652111	-0.312656
12	7	0	1.239773	2.300628	-0.561950
13	7	0	0.872786	-1.083148	-0.322210
14	1	0	0.968598	-2.065425	-0.559988
15	1	0	2.025613	1.916909	0.099543
16	6	0	2.190228	-0.572425	0.211617
17	8	0	3.119473	-1.295618	-0.086913

18	8	0	2.098441	0.482743	0.894416

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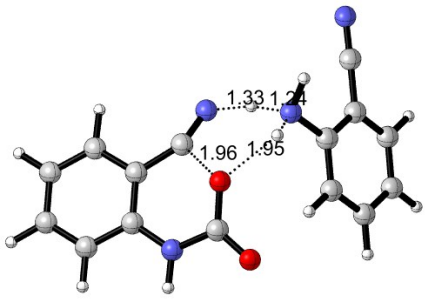
b-**TS$_{3/4}$'**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.431184	-0.671910	0.486820
2	6	0	3.084699	-0.529519	0.106944
3	6	0	2.542598	0.770927	0.079298
4	6	0	3.338606	1.878665	0.414262
5	6	0	4.665570	1.719960	0.774336
6	6	0	5.203962	0.429228	0.814503
7	1	0	4.862497	-1.669128	0.514569
8	1	0	2.882021	2.863487	0.385556
9	1	0	5.272620	2.582715	1.025942
10	1	0	6.241665	0.281324	1.099407
11	6	0	1.153715	1.049619	-0.203994
12	7	0	0.218416	1.773450	-0.148217
13	7	0	2.349775	-1.658710	-0.184781
14	1	0	2.763660	-2.563685	-0.003437
15	6	0	1.113235	-1.704185	-0.854664
16	8	0	0.584437	-2.796664	-1.034588
17	8	0	0.655626	-0.554833	-1.207569
18	1	0	-0.884540	1.322327	-0.728222
19	1	0	-1.116932	-0.006017	-1.815475
20	7	0	-1.744988	0.641203	-1.316108
21	1	0	-2.286029	1.220338	-1.961505
22	6	0	-2.563057	-0.075213	-0.372872
23	6	0	-2.246817	-1.385250	-0.030443
24	6	0	-3.638248	0.581122	0.242602
25	6	0	-4.402985	-0.083118	1.206587
26	6	0	-4.083916	-1.390009	1.556122
27	6	0	-3.012651	-2.033779	0.936720
28	6	0	-3.948724	1.927264	-0.154969
29	1	0	-5.235650	0.434712	1.671166
30	1	0	-4.672716	-1.906115	2.307306

31	1	0	-2.764229	-3.056731	1.201796
32	1	0	-1.413345	-1.895362	-0.512054
33	7	0	-4.164998	3.001387	-0.530223

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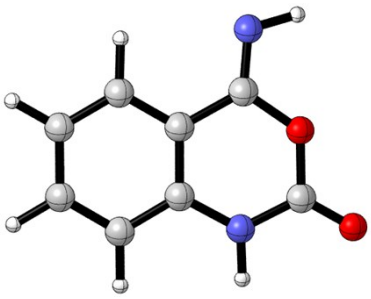
b-**4**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.764385	1.182534	-0.000239
2	6	0	2.915391	0.407293	-0.000281
3	6	0	2.810326	-0.987821	-0.000076
4	6	0	1.567899	-1.607656	0.000146
5	6	0	0.508496	0.571135	-0.000020
6	6	0	0.413430	-0.820932	0.000165
7	6	0	-0.726638	1.367102	0.000126
8	7	0	-0.744760	2.627866	0.000636
9	7	0	-0.854703	-1.397785	0.000415
10	1	0	-1.704492	2.978283	0.000501
11	1	0	1.805090	2.267095	-0.000359
12	1	0	3.891530	0.880680	-0.000473
13	1	0	3.707751	-1.599002	-0.000105
14	1	0	1.486405	-2.691110	0.000298
15	1	0	-0.958266	-2.404361	0.000798
16	6	0	-2.035856	-0.702373	-0.000118
17	8	0	-3.119613	-1.219938	-0.000033
18	8	0	-1.922434	0.657709	-0.000746

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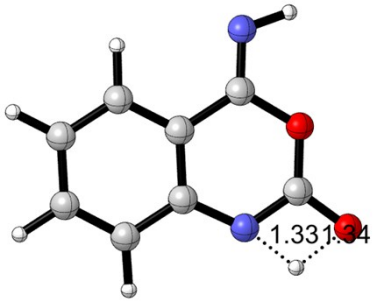
b-**TS$_{4/5}$**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.393922	-0.838582	-0.000179
2	1	0	-1.956371	-2.171551	0.000051

3	6	0	-1.946870	-0.607937	-0.000094
4	8	0	-1.948526	0.712841	0.000008
5	1	0	-1.664385	3.030186	-0.000233
6	6	0	-0.708923	1.399840	-0.000085
7	7	0	-0.713729	2.657314	-0.000204
8	6	0	0.502169	0.562837	0.000024
9	7	0	-0.882430	-1.384635	-0.000481
10	8	0	-2.991182	-1.325623	0.000276
11	6	0	1.765016	1.162188	0.000289
12	1	0	1.821880	2.246199	0.000439
13	6	0	2.907294	0.374172	0.000354
14	6	0	1.543564	-1.631728	-0.000139
15	1	0	1.439780	-2.711899	-0.000324
16	6	0	2.790130	-1.021005	0.000137
17	1	0	3.887678	0.839073	0.000574
18	1	0	3.684384	-1.637222	0.000178

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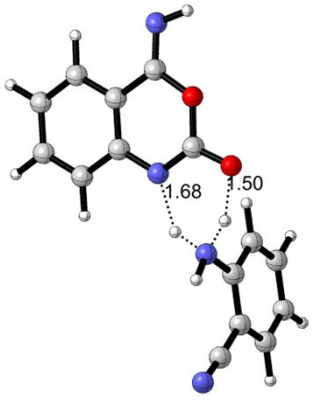
b-**TS$_{4/5}$'**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.665310	-0.297440	-1.149011
2	1	0	-4.231588	-3.001639	0.082794
3	6	0	-1.974333	0.697349	-0.184247
4	6	0	-1.856249	2.093334	-0.095116
5	6	0	-2.953681	2.865910	0.252526
6	6	0	-4.193826	2.270247	0.520682
7	6	0	-3.217624	0.107696	0.086045
8	6	0	-4.320900	0.892244	0.436796
9	1	0	-5.047986	2.882553	0.791159
10	1	0	-2.847889	3.945461	0.316278
11	7	0	-0.867461	-0.064389	-0.532770
12	1	0	-5.264350	0.393055	0.635529
13	6	0	-0.989081	-1.378870	-0.623877
14	8	0	-0.044601	-2.151416	-0.928210
15	8	0	-2.170974	-2.017913	-0.378473



16	1	0	-0.892870	2.550607	-0.303362
17	6	0	-3.329227	-1.350055	-0.010975
18	7	0	-4.389462	-2.001080	0.214989
19	1	0	0.730245	0.228189	-0.957555
20	1	0	1.142797	-1.280353	-1.191970
21	1	0	2.089729	-0.025997	-2.038509
22	6	0	2.559200	-0.212088	-0.023738
23	6	0	2.118323	-0.676510	1.210577
24	6	0	2.964460	-0.592076	2.312506
25	6	0	4.244835	-0.050305	2.188905
26	6	0	4.686425	0.412202	0.955887
27	6	0	3.841171	0.334380	-0.157009
28	1	0	2.619470	-0.956317	3.274878
29	1	0	4.898547	0.008375	3.052718
30	1	0	5.678415	0.835366	0.837501
31	6	0	4.264987	0.803497	-1.447904
32	1	0	1.123462	-1.104200	1.294269
33	7	0	4.543005	1.159738	-2.514152

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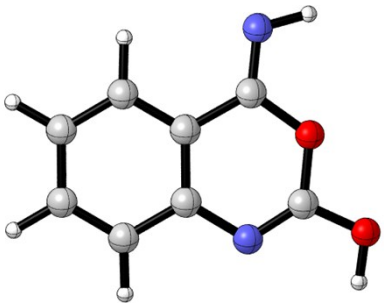
b-**5**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398901	-0.834601	-0.000084
2	1	0	3.074267	-2.088751	0.000200
3	6	0	1.868139	-0.671699	-0.000486
4	8	0	1.881796	0.669970	0.000048
5	1	0	1.658523	3.000420	-0.000083
6	6	0	0.679675	1.385054	0.000139
7	7	0	0.700987	2.645439	-0.000045
8	6	0	-0.532894	0.560854	0.000075
9	7	0	0.859480	-1.448177	-0.000363
10	8	0	3.121121	-1.117814	0.000062
11	6	0	-1.799122	1.153489	0.000228
12	1	0	-1.865091	2.236993	0.000362
13	6	0	-2.932373	0.353557	0.000264

14	6	0	-1.546897	-1.634552	-0.000055
15	1	0	-1.425684	-2.713098	-0.000187
16	6	0	-2.801147	-1.041265	0.000109
17	1	0	-3.918184	0.807748	0.000426
18	1	0	-3.689314	-1.666411	0.000130

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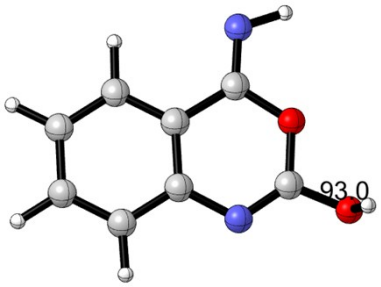
b-$TS_{5/6}$



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.407381	-0.833285	-0.005788
2	1	0	3.497457	-1.295306	0.802891
3	6	0	1.863843	-0.699001	-0.014382
4	8	0	1.871738	0.657407	-0.004861
5	1	0	1.658690	2.993911	-0.008178
6	6	0	0.678960	1.379457	-0.002733
7	7	0	0.700302	2.641024	-0.001720
8	6	0	-0.538135	0.561261	0.000392
9	7	0	0.849662	-1.456701	-0.013908
10	8	0	3.121118	-1.172894	-0.082062
11	6	0	-1.803130	1.155283	0.008140
12	1	0	-1.869121	2.238729	0.011586
13	6	0	-2.936445	0.354557	0.010728
14	6	0	-1.554157	-1.634095	-0.003730
15	1	0	-1.430874	-2.712365	-0.010290
16	6	0	-2.808426	-1.040384	0.004975
17	1	0	-3.921910	0.809765	0.016970
18	1	0	-3.697618	-1.663860	0.006185

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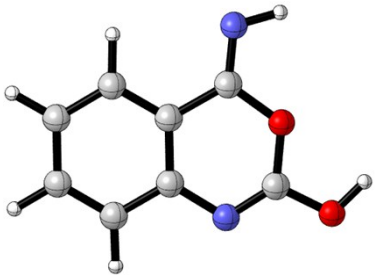
b-**6**



Standard orientation:

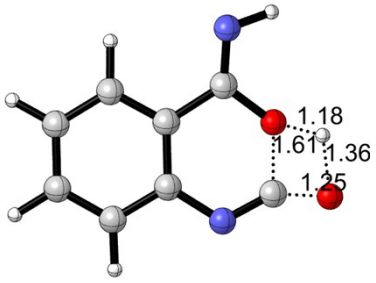
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.416759	-0.838532	-0.000066
2	1	0	-3.724487	-0.521514	0.000118
3	6	0	-1.846518	-0.737724	0.000065
4	8	0	-1.882999	0.620778	0.000330
5	1	0	-1.703450	2.965070	-0.000185
6	6	0	-0.695535	1.363792	-0.000082
7	7	0	-0.741165	2.623922	-0.000271
8	6	0	0.528595	0.559435	-0.000026
9	7	0	-0.824499	-1.484193	-0.000140
10	8	0	-3.077541	-1.244942	0.000006
11	6	0	1.784848	1.174008	0.000042
12	1	0	1.832829	2.258360	0.000060
13	6	0	2.931155	0.393585	0.000077
14	6	0	1.579635	-1.617644	-0.000036
15	1	0	1.474810	-2.697702	-0.000075
16	6	0	2.823303	-1.003568	0.000039
17	1	0	3.909014	0.864494	0.000136
18	1	0	3.721798	-1.613622	0.000068

b-$\mathbf{TS_{6/7}}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.452742	-0.862105	-0.020104
2	1	0	-2.919942	0.208385	0.093222
3	6	0	-1.829000	-1.040249	0.000706
4	8	0	-1.836674	0.513926	0.438836
5	1	0	-1.853536	2.889537	-0.127947
6	6	0	-0.786468	1.326094	0.011622
7	7	0	-0.897181	2.552486	-0.246197
8	6	0	0.469312	0.547910	-0.005147
9	7	0	-0.732913	-1.616966	-0.117558
10	8	0	-3.067925	-1.118138	-0.143231
11	6	0	1.688136	1.231287	0.005714
12	1	0	1.667609	2.316798	0.007893



13	6	0	2.886784	0.530889	0.021735
14	6	0	1.664082	-1.556745	-0.007169
15	1	0	1.632053	-2.641161	-0.028375
16	6	0	2.869277	-0.866305	0.020113
17	1	0	3.829466	1.068230	0.037357
18	1	0	3.802613	-1.421389	0.034484

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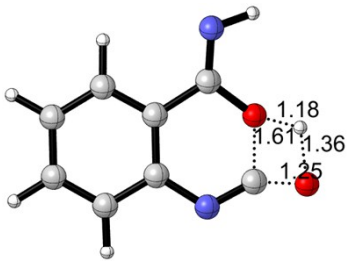
b-**TS$_{6/7}$'**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.661016	-0.020107	-1.249780
2	1	0	-0.091980	2.102662	0.690755
3	6	0	3.216251	-0.658287	-0.204299
4	6	0	4.589403	-0.952534	-0.200410
5	6	0	5.509107	-0.038127	0.288062
6	6	0	5.084689	1.199122	0.788389
7	6	0	2.794654	0.586083	0.300403
8	6	0	3.732507	1.502574	0.791891
9	1	0	5.805883	1.914069	1.171729
10	1	0	6.566843	-0.286615	0.280477
11	7	0	2.366715	-1.628350	-0.728299
12	1	0	-1.416138	-0.850748	-1.807631
13	1	0	3.366204	2.450352	1.173605
14	6	0	1.112808	-1.503171	-0.791978
15	8	0	0.124639	-2.085032	-1.188841
16	8	0	0.551750	-0.069226	-0.121202
17	1	0	4.901951	-1.914395	-0.594332
18	6	0	1.364767	0.934843	0.317733
19	7	0	0.928489	2.059171	0.722269
20	1	0	-0.629880	0.132321	-0.684523
21	6	0	-2.706401	-0.322044	-0.296526
22	6	0	-2.630786	-1.499657	0.437028
23	6	0	-3.617866	-1.769117	1.382624
24	6	0	-4.663017	-0.870717	1.602068
25	6	0	-3.746509	0.589509	-0.081443

26	6	0	-4.730094	0.310107	0.873632
27	1	0	-1.803581	-2.182923	0.259160
28	1	0	-3.565004	-2.689414	1.955552
29	1	0	-5.424846	-1.089522	2.342896
30	1	0	-5.532840	1.022803	1.030392
31	6	0	-3.785503	1.794616	-0.863842
32	1	0	-1.894513	0.766889	-1.860988
33	7	0	-3.753799	2.737770	-1.535151

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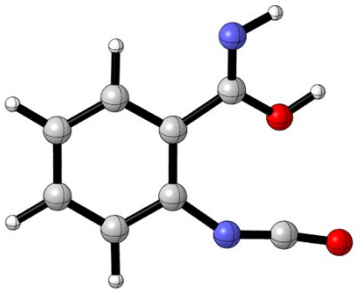
b-7



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.313595	-0.848062	-0.020136
2	1	0	-2.411296	1.757559	0.562266
3	6	0	-2.122950	-1.290610	-0.114340
4	8	0	-1.697353	1.103915	0.625033
5	1	0	-1.201353	3.321606	-0.372417
6	6	0	-0.570095	1.558357	0.011956
7	7	0	-0.389035	2.711417	-0.484285
8	6	0	0.519502	0.545384	0.010783
9	7	0	-0.933479	-1.458811	-0.108568
10	8	0	-3.294442	-1.270038	-0.142428
11	6	0	1.832560	1.029181	0.032548
12	1	0	1.970085	2.105435	0.037841
13	6	0	2.922653	0.169990	0.049494
14	6	0	1.416261	-1.709886	-0.007881
15	1	0	1.227403	-2.777807	-0.039628
16	6	0	2.709485	-1.208237	0.033813
17	1	0	3.930379	0.571977	0.075911
18	1	0	3.550665	-1.894731	0.047739

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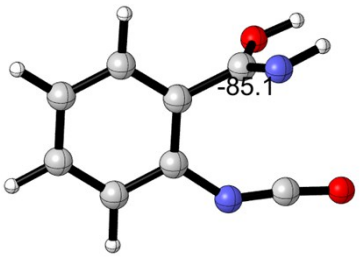
b-$TS_{7/8}$

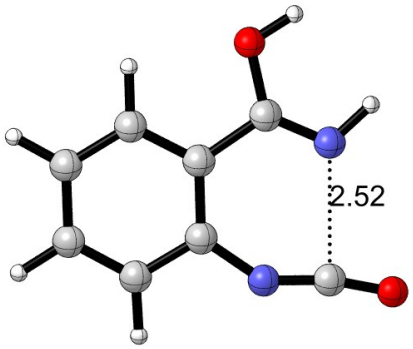


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.463365	-0.833698	0.006464
2	6	0	-1.915716	-1.373656	0.002348
3	8	0	-1.254635	1.625830	1.158395
4	1	0	-2.349260	1.955210	-1.068426
5	6	0	-0.845721	1.288585	-0.093431
6	7	0	-1.450391	1.479478	-1.188951
7	6	0	0.459038	0.566525	-0.050792
8	7	0	-0.725263	-1.567473	0.036541
9	8	0	-3.085673	-1.318797	-0.006783
10	6	0	1.667335	1.256730	-0.070215
11	1	0	1.653728	2.341884	-0.117386
12	6	0	2.876011	0.565353	-0.039402
13	6	0	1.672139	-1.528199	0.038497
14	1	0	1.649893	-2.612171	0.081040
15	6	0	2.873483	-0.827607	0.015367
16	1	0	3.813428	1.111873	-0.059451
17	1	0	3.811258	-1.374260	0.039554
18	1	0	-2.126613	2.052969	1.125624

b-**8**

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.213539	-0.885782	-0.000238
2	6	0	2.241634	-1.188519	-0.000345
3	8	0	-0.022148	2.797159	-0.000992
4	1	0	2.366812	2.103462	0.000877
5	6	0	0.520167	1.549053	0.000016
6	7	0	1.762112	1.280860	0.001018
7	6	0	-0.520491	0.494336	0.000065
8	7	0	1.058100	-1.431720	-0.000842
9	8	0	3.410859	-1.180392	0.000062
10	6	0	-1.869579	0.879150	0.000463

11	1	0	-2.102739	1.937396	0.000675
12	6	0	-2.896332	-0.054027	0.000611
13	6	0	-1.259733	-1.818650	-0.000137
14	1	0	-0.993729	-2.870528	-0.000428
15	6	0	-2.585385	-1.413549	0.000313
16	1	0	-3.929817	0.277391	0.000945
17	1	0	-3.375363	-2.158999	0.000407
18	1	0	0.683201	3.461096	-0.000751

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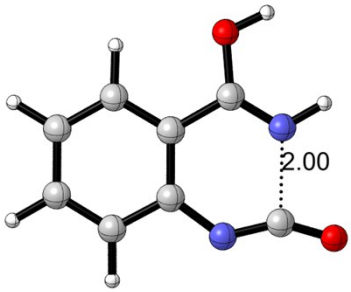
b-$\mathbf{TS_{8/9}}$



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.297872	-0.891214	0.000005
2	6	0	-2.085662	-1.081716	-0.000005
3	8	0	-0.360890	2.714099	-0.000012
4	1	0	-2.643572	1.529662	-0.000020
5	6	0	-0.659866	1.400098	-0.000009
6	7	0	-1.838809	0.905403	-0.000013
7	6	0	0.495732	0.509774	0.000001
8	7	0	-0.919281	-1.538304	0.000003
9	8	0	-3.252965	-1.240222	-0.000009
10	6	0	1.795658	1.040784	0.000004
11	1	0	1.917799	2.118605	0.000000
12	6	0	2.901196	0.209235	0.000012
13	6	0	1.437218	-1.717109	0.000014
14	1	0	1.276804	-2.790169	0.000017
15	6	0	2.711759	-1.178774	0.000017
16	1	0	3.901625	0.629260	0.000015
17	1	0	3.571317	-1.842883	0.000023
18	1	0	-1.169944	3.248362	-0.000022

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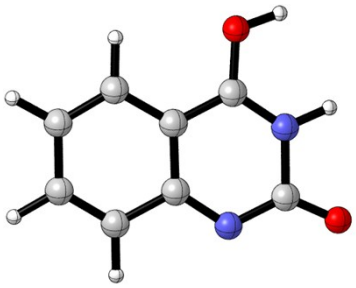
b-**9**



Standard orientation:

1	6	0	0.340456	-0.891042	0.000003
2	6	0	-1.980478	-0.864837	-0.000028
3	8	0	-0.683752	2.592199	-0.000009
4	1	0	-2.760962	1.068031	-0.000018
5	6	0	-0.709454	1.258632	-0.000010
6	7	0	-1.860354	0.596762	-0.000016
7	6	0	0.487072	0.535880	-0.000004
8	7	0	-0.824123	-1.547807	-0.000001
9	8	0	-3.121116	-1.285893	0.000011
10	6	0	1.765694	1.161072	0.000002
11	1	0	1.822270	2.245297	-0.000002
12	6	0	2.892798	0.389767	0.000013
13	6	0	1.553769	-1.652219	0.000016
14	1	0	1.457979	-2.732940	0.000022
15	6	0	2.772124	-1.031949	0.000020
16	1	0	3.875605	0.849115	0.000018
17	1	0	3.675843	-1.635357	0.000030
18	1	0	-1.572350	2.980900	-0.000011

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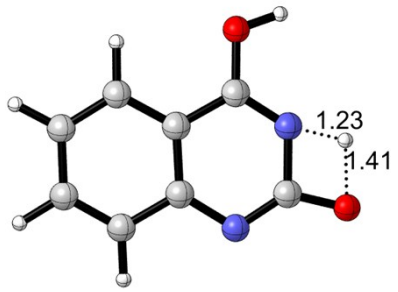
b-$TS_{9/10}$

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.394902	-0.898606	0.000029
2	6	0	1.861840	-0.892279	0.000009
3	8	0	0.788297	2.553184	-0.000079
4	1	0	3.071845	0.226385	-0.000033
5	6	0	0.774048	1.223890	-0.000041
6	7	0	1.875403	0.523388	-0.000032
7	6	0	-0.469674	0.525891	-0.000010
8	7	0	0.772851	-1.611337	0.000039
9	8	0	3.104348	-1.185413	0.000008
10	6	0	-1.711498	1.199347	-0.000018
11	1	0	-1.722800	2.285062	-0.000048
12	6	0	-2.879154	0.474431	0.000011
13	6	0	-1.620848	-1.609320	0.000059

14	1	0	-1.570109	-2.693141	0.000088
15	6	0	-2.822288	-0.939219	0.000050
16	1	0	-3.838914	0.980404	0.000005
17	1	0	-3.748298	-1.507424	0.000073
18	1	0	1.704189	2.877381	-0.000097

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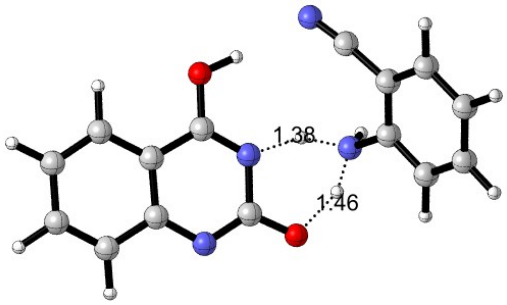
b-**TS$_{9/10}$'**

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.270734	-1.505459	-1.266432
2	6	0	-2.983277	-0.916904	0.129415
3	6	0	-0.852160	-1.448523	-0.547062
4	8	0	-1.142410	2.142641	-0.410099
5	6	0	-1.428030	0.844672	-0.335284
6	7	0	-0.524377	-0.063237	-0.621375
7	6	0	-2.742147	0.480355	0.065112
8	7	0	-2.054381	-1.854614	-0.171819
9	8	0	0.080426	-2.252573	-0.864274
10	6	0	-3.746168	1.422766	0.385906
11	1	0	-3.515511	2.481788	0.322640
12	6	0	-4.989208	0.983409	0.771264
13	6	0	-4.281867	-1.334931	0.533412
14	1	0	-4.472039	-2.402274	0.584326
15	6	0	-5.248031	-0.409067	0.842716
16	1	0	-5.770931	1.693891	1.020338
17	1	0	-6.233818	-0.748801	1.149450
18	1	0	-0.211084	2.304704	-0.657709
19	1	0	0.788406	0.004935	-1.028359
20	7	0	1.836032	-0.542983	-1.350101
21	1	0	2.109753	-0.321642	-2.308193
22	6	0	2.906251	-0.419713	-0.407944
23	6	0	3.576915	-1.538767	0.072830
24	6	0	3.254849	0.850874	0.077590
25	6	0	4.289019	1.006932	1.004807
26	6	0	4.966074	-0.117742	1.462048

27	6	0	4.602892	-1.384593	1.003802
28	6	0	2.466690	1.962098	-0.376501
29	7	0	1.752632	2.786793	-0.765504
30	1	0	5.766672	-0.007315	2.185822
31	1	0	5.120947	-2.263270	1.375540
32	1	0	3.281439	-2.522713	-0.279334
33	1	0	4.541149	1.998688	1.365820

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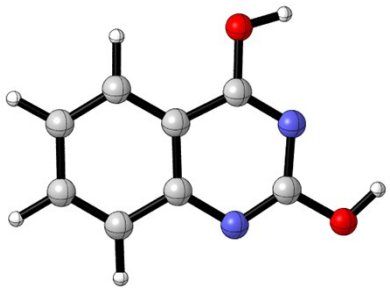
b-**10**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.372916	-0.871090	-0.000064
2	6	0	1.879325	-0.696512	-0.000142
3	8	0	0.674512	2.589262	0.000116
4	1	0	3.753178	-0.564108	0.000125
5	6	0	0.725183	1.252837	-0.000162
6	7	0	1.892611	0.667182	-0.000092
7	6	0	-0.507648	0.537089	-0.000056
8	7	0	0.846913	-1.486309	-0.000128
9	8	0	3.090652	-1.272830	0.000107
10	6	0	-1.779432	1.150818	0.000066
11	1	0	-1.845542	2.234247	0.000080
12	6	0	-2.906658	0.362898	0.000121
13	6	0	-1.550518	-1.657223	-0.000005
14	1	0	-1.442257	-2.736922	-0.000018
15	6	0	-2.783753	-1.047289	0.000081
16	1	0	-3.891932	0.818080	0.000194
17	1	0	-3.682397	-1.657545	0.000137
18	1	0	1.589461	2.919502	0.000203

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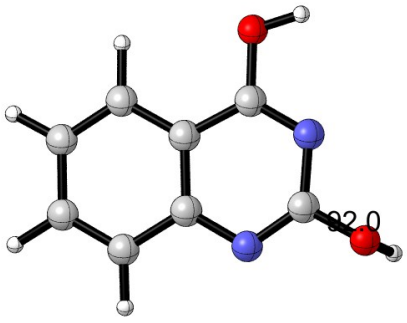
b-**TS$_{10/11}$**



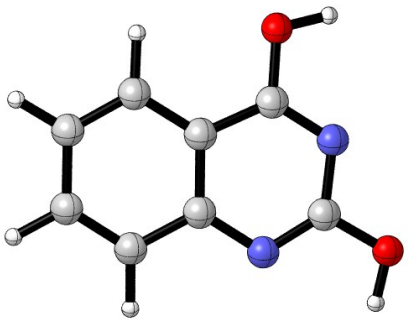
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.360634	-0.864875	-0.003673
2	6	0	-1.897827	-0.650391	-0.015686
3	8	0	-0.630475	2.609529	0.007013
4	1	0	-3.499975	-1.349989	0.798829
5	6	0	-0.703921	1.273516	-0.001384
6	7	0	-1.881181	0.709130	-0.006042
7	6	0	0.518576	0.538971	-0.002603
8	7	0	-0.875207	-1.453923	-0.010308
9	8	0	-3.140435	-1.202008	-0.087858
10	6	0	1.801625	1.128394	0.001410
11	1	0	1.888935	2.210300	0.000867
12	6	0	2.912720	0.317384	0.006048
13	6	0	1.520329	-1.676116	0.001090
14	1	0	1.390069	-2.753537	-0.001195
15	6	0	2.765395	-1.090348	0.006286
16	1	0	3.906714	0.753661	0.009257
17	1	0	3.653040	-1.716398	0.009329
18	1	0	-1.541965	2.950130	-0.004811

b-**11**

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.352632	-0.865603	-0.000078
2	6	0	-1.904754	-0.629452	-0.000043
3	8	0	-0.628183	2.612721	0.000240
4	1	0	-3.037230	-2.115385	0.000310
5	6	0	-0.709442	1.278440	-0.000523
6	7	0	-1.891192	0.725625	-0.000191
7	6	0	0.512436	0.538585	-0.000204
8	7	0	-0.885644	-1.446138	-0.000039
9	8	0	-3.140011	-1.149272	0.000217
10	6	0	1.795210	1.126719	-0.000037
11	1	0	1.881847	2.208681	-0.000132

12	6	0	2.907808	0.316997	0.000094
13	6	0	1.512394	-1.675764	0.000091
14	1	0	1.385152	-2.753507	0.000187
15	6	0	2.757952	-1.089648	0.000156
16	1	0	3.901674	0.753007	0.000137
17	1	0	3.644456	-1.717407	0.000295
18	1	0	-1.537922	2.958969	0.000425

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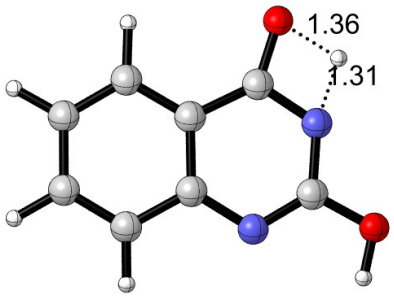
b-$TS_{11/12}$



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.395523	-0.826249	-0.000004
2	6	0	1.887724	-0.673098	-0.000083
3	6	0	0.666250	1.319816	0.000007
4	6	0	-0.556893	0.583705	0.000034
5	7	0	0.835765	-1.441159	-0.000064
6	8	0	3.111224	-1.204874	-0.000140
7	6	0	-1.830467	1.181973	0.000094
8	1	0	-1.900704	2.265671	0.000122
9	6	0	-2.951520	0.381010	0.000115
10	6	0	-1.563052	-1.620554	0.000019
11	1	0	-1.449380	-2.699747	-0.000011
12	6	0	-2.806545	-1.023354	0.000077
13	1	0	-3.942541	0.823019	0.000163
14	1	0	-3.695577	-1.647706	0.000093
15	7	0	1.847318	0.676483	-0.000050
16	8	0	0.934115	2.566222	0.000024
17	1	0	2.145707	1.951702	-0.000033
18	1	0	2.998359	-2.170485	-0.000159

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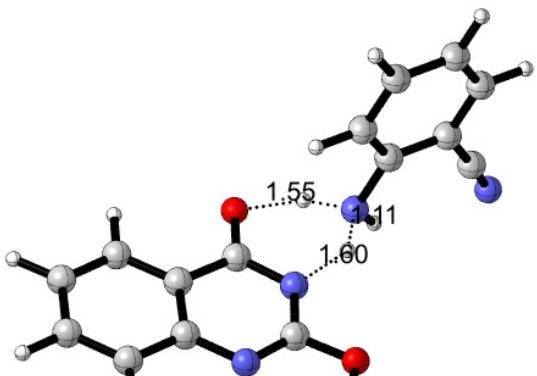
b-$TS_{11/12}$'



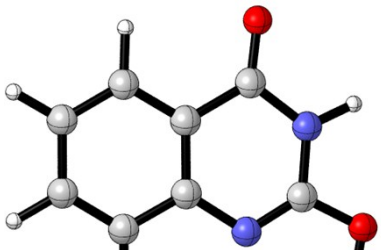
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	-0.890681	0.912516	-0.561571
2	6	0	3.317881	0.522537	0.384394
3	6	0	1.414656	1.720053	0.651528
4	6	0	1.218217	-0.190278	-0.657625
5	6	0	2.636339	-0.415861	-0.417831
6	7	0	2.681862	1.615438	0.929487
7	8	0	0.734167	2.769584	1.155301
8	6	0	3.308997	-1.522562	-0.963242
9	1	0	2.743638	-2.217016	-1.577611
10	6	0	4.655018	-1.699497	-0.713358
11	6	0	4.693997	0.325329	0.629050
12	1	0	5.214675	1.051263	1.246049
13	6	0	5.343407	-0.766086	0.088314
14	1	0	5.184095	-2.550162	-1.131848
15	1	0	6.403243	-0.907898	0.282504
16	7	0	0.644356	0.902689	-0.093602
17	8	0	0.524263	-0.983977	-1.361163
18	1	0	1.376076	3.291063	1.665131
19	1	0	-0.912649	-0.402199	-1.445066
20	7	0	-1.664127	0.310152	-1.081200
21	1	0	-2.124607	0.827568	-1.832923
22	6	0	-2.574302	-0.297242	-0.147161
23	6	0	-2.057681	-1.141438	0.829918
24	6	0	-3.948110	-0.034716	-0.199495
25	6	0	-4.808212	-0.623961	0.734317
26	6	0	-4.291225	-1.464331	1.711668
27	6	0	-2.920086	-1.721315	1.755812
28	6	0	-4.452144	0.837703	-1.224734
29	1	0	-5.871215	-0.413386	0.680542
30	1	0	-4.956948	-1.920512	2.436759
31	1	0	-2.516003	-2.381985	2.516245
32	1	0	-0.990245	-1.342308	0.848383
33	7	0	-4.797426	1.542892	-2.075973

b-**12**

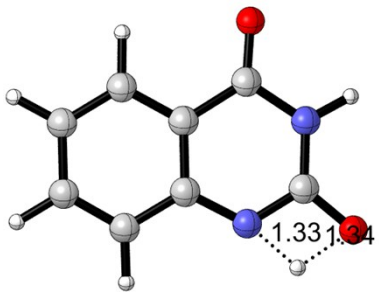
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.365821	-0.839520	-0.000195
2	6	0	-1.898766	-0.642081	0.000050
3	6	0	-0.636723	1.434269	-0.000675
4	6	0	0.542068	0.557819	-0.000269
5	7	0	-0.891788	-1.436494	-0.000098
6	8	0	-3.157392	-1.100660	0.000418
7	6	0	1.825251	1.119535	-0.000059
8	1	0	1.914091	2.201934	-0.000124
9	6	0	2.937090	0.295884	0.000091
10	6	0	1.504174	-1.662679	-0.000038
11	1	0	1.360567	-2.738558	0.000031
12	6	0	2.768325	-1.098488	0.000093
13	1	0	3.934855	0.723027	0.000186
14	1	0	3.641543	-1.744641	0.000234
15	7	0	-1.840752	0.721435	-0.000170
16	8	0	-0.637670	2.649203	0.000427
17	1	0	-2.701973	1.258556	0.000303
18	1	0	-3.104253	-2.071685	0.000502

b-$\mathbf{TS_{12/13}}$

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.360442	-0.842056	-0.000004
2	6	0	1.981429	-0.577996	-0.000080
3	6	0	0.666620	1.448069	0.000004
4	6	0	-0.512506	0.560508	0.000029
5	7	0	0.917766	-1.366590	-0.000059
6	8	0	3.026700	-1.310520	-0.000129
7	6	0	-1.792442	1.127477	0.000084
8	1	0	-1.874128	2.210433	0.000109
9	6	0	-2.912412	0.313093	0.000107

10	6	0	-1.497091	-1.661703	0.000019
11	1	0	-1.369107	-2.739354	-0.000007
12	6	0	-2.755223	-1.081346	0.000074
13	1	0	-3.905995	0.748896	0.000152
14	1	0	-3.633701	-1.720145	0.000091
15	7	0	1.905179	0.769155	-0.000051
16	8	0	0.645169	2.659594	0.000028
17	1	0	2.751349	1.329409	-0.000071
18	1	0	1.988422	-2.156063	-0.000109

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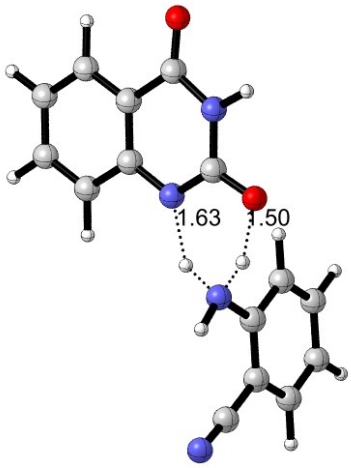
b-$TS_{11/12}$'

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.654714	-0.330760	-1.128773
2	6	0	-1.957853	0.672924	-0.184901
3	6	0	-0.993220	-1.422359	-0.589370
4	6	0	-3.389276	-1.343324	0.008496
5	6	0	-3.222495	0.114338	0.083796
6	7	0	-0.858473	-0.097948	-0.513843
7	8	0	-0.031451	-2.200233	-0.882424
8	6	0	-4.314254	0.925836	0.415509
9	1	0	-5.267665	0.443522	0.611335
10	6	0	-4.163721	2.299612	0.483825
11	6	0	-1.821325	2.072543	-0.109992
12	1	0	-0.849022	2.512515	-0.314360
13	6	0	-2.906476	2.866384	0.217856
14	1	0	-5.006519	2.933493	0.739643
15	1	0	-2.780678	3.944548	0.269204
16	7	0	-2.217222	-2.010457	-0.333410
17	8	0	-4.421101	-1.956247	0.215532
18	1	0	-2.263805	-3.021202	-0.411014
19	1	0	1.149606	-1.323932	-1.157885
20	1	0	0.695658	0.174732	-0.927191
21	6	0	2.560215	-0.216642	-0.018045
22	6	0	2.138053	-0.659965	1.231090

23	6	0	3.837150	0.336178	-0.175189
24	6	0	2.995971	-0.549202	2.321210
25	6	0	4.271161	-0.000982	2.172767
26	6	0	4.694525	0.441272	0.926199
27	1	0	1.147083	-1.092397	1.334625
28	1	0	2.664680	-0.897350	3.294353
29	1	0	4.934645	0.078767	3.027421
30	1	0	5.681987	0.869246	0.788461
31	6	0	4.243968	0.783203	-1.479323
32	7	0	4.509335	1.120538	-2.554956
33	1	0	2.061424	-0.058637	-2.026146

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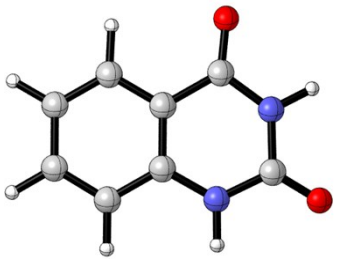
b-**13** (2a)

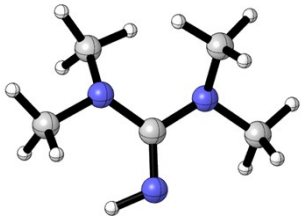


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.386350	-0.827921	-0.000001
2	6	0	2.061955	-0.675333	-0.000088
3	6	0	0.690845	1.414416	0.000011
4	6	0	-0.517777	0.565880	0.000033
5	7	0	0.884242	-1.389540	-0.000057
6	8	0	3.156343	-1.199827	-0.000144
7	6	0	-1.786199	1.151663	0.000087
8	1	0	-1.845863	2.235827	0.000111
9	6	0	-2.920984	0.355910	0.000108
10	6	0	-1.531152	-1.633795	0.000021
11	1	0	-1.431259	-2.715658	-0.000005
12	6	0	-2.783594	-1.037767	0.000074
13	1	0	-3.907671	0.806511	0.000151
14	1	0	-3.668365	-1.667187	0.000090
15	7	0	1.887675	0.701608	-0.000048
16	8	0	0.686969	2.628073	0.000029
17	1	0	2.743741	1.247039	-0.000071
18	1	0	0.999041	-2.395292	-0.000089

4.2 TMG-catalyzed reaction

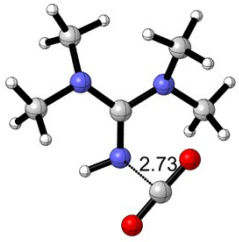
TMG



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.157178	-0.228143	0.129984
2	6	0	-0.011904	0.538750	-0.011247
3	7	0	-1.171240	-0.225054	-0.139670
4	7	0	-0.086527	1.819668	-0.019503
5	6	0	2.367846	0.489518	0.469334
6	6	0	1.385481	-1.299562	-0.832828
7	6	0	-1.377519	-1.319553	0.800313
8	6	0	-2.387627	0.524512	-0.404937
9	1	0	0.836345	2.245851	-0.076017
10	1	0	2.181634	1.160224	1.311695
11	1	0	2.768630	1.075197	-0.376016
12	1	0	3.129915	-0.235766	0.768499
13	1	0	0.438072	-1.750553	-1.126808
14	1	0	2.024421	-2.066480	-0.382158
15	1	0	1.883623	-0.919771	-1.739301
16	1	0	-1.809341	-0.953480	1.745415
17	1	0	-2.069798	-2.045772	0.362609
18	1	0	-3.168611	-0.183643	-0.697758
19	1	0	-2.213027	1.235103	-1.212550
20	1	0	-2.720930	1.089146	0.478172
21	1	0	-0.434474	-1.817339	1.024727

TMG-**1**

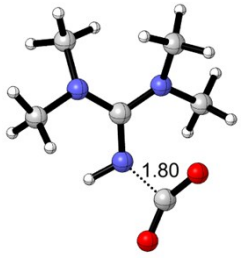


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.392610	-0.874310	-0.206185
2	6	0	0.496169	-0.049309	0.486787
3	7	0	0.648685	1.300671	0.224853

4	7	0	-0.427594	-0.444842	1.293576
5	6	0	1.154019	-2.301793	-0.147509
6	6	0	2.809588	-0.531104	-0.186869
7	6	0	0.853366	1.763519	-1.140694
8	6	0	-0.113906	2.224262	1.045797
9	1	0	-0.317840	-1.426620	1.540025
10	1	0	0.101043	-2.517088	-0.346782
11	1	0	1.431980	-2.740791	0.825677
12	1	0	1.755950	-2.787117	-0.921045
13	1	0	2.935909	0.548836	-0.116368
14	1	0	3.287612	-0.887908	-1.105398
15	1	0	3.315988	-0.996417	0.673262
16	1	0	-0.098164	2.098595	-1.577107
17	1	0	1.557827	2.603525	-1.149150
18	1	0	0.339837	3.216251	0.954351
19	1	0	-0.083428	1.899724	2.085816
20	1	0	-1.164294	2.279513	0.729137
21	1	0	1.249866	0.958444	-1.759671
22	6	0	-2.562782	-0.395460	-0.402277
23	8	0	-2.972094	-1.397130	0.023578
24	8	0	-2.206271	0.599595	-0.892311

TMG-**TS$_{1/2}$**

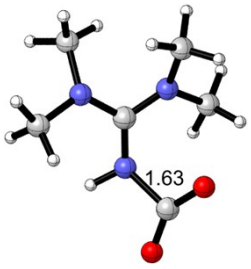


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.490604	-0.827826	0.060714
2	6	0	-0.378893	-0.106821	-0.290329
3	7	0	-0.458876	1.243230	-0.190522
4	7	0	0.738957	-0.664955	-0.695307
5	6	0	-1.371443	-2.252244	0.316297
6	6	0	-2.835049	-0.360058	-0.241988
7	6	0	-1.140202	1.887853	0.921328
8	6	0	0.466227	2.102847	-0.915816
9	1	0	0.669889	-1.638082	-0.976645
10	1	0	-0.425613	-2.463839	0.818964

11	1	0	-1.434506	-2.845620	-0.607583
12	1	0	-2.189738	-2.555820	0.975089
13	1	0	-2.792184	0.631772	-0.692451
14	1	0	-3.449484	-0.316008	0.664805
15	1	0	-3.312307	-1.046116	-0.953167
16	1	0	-0.397657	2.414185	1.532752
17	1	0	-1.879851	2.611830	0.558922
18	1	0	-0.088097	2.981794	-1.262939
19	1	0	0.866834	1.560098	-1.771976
20	1	0	1.295460	2.412647	-0.273743
21	1	0	-1.637089	1.144905	1.545409
22	6	0	2.280488	-0.421079	0.208176
23	8	0	2.170745	0.571314	0.877552
24	8	0	2.969409	-1.352299	-0.098507

TMG-**2**



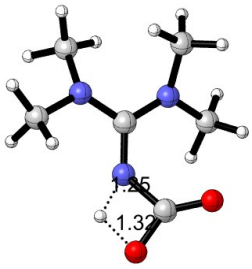
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.490962	-0.819805	0.031478
2	6	0	-0.362093	-0.107152	-0.245775
3	7	0	-0.422880	1.236981	-0.173277
4	7	0	0.769065	-0.706235	-0.579850
5	6	0	-1.402413	-2.233545	0.360330
6	6	0	-2.816947	-0.339342	-0.327939
7	6	0	-1.182112	1.912346	0.868932
8	6	0	0.540416	2.082866	-0.868005
9	1	0	0.708004	-1.663961	-0.907869
10	1	0	-0.473167	-2.434667	0.896193
11	1	0	-1.452844	-2.867127	-0.536118
12	1	0	-2.242644	-2.490765	1.011134
13	1	0	-2.740113	0.624779	-0.831213
14	1	0	-3.453553	-0.233327	0.558178
15	1	0	-3.288055	-1.054863	-1.012358
16	1	0	-0.482010	2.472847	1.498254

17	1	0	-1.909465	2.608823	0.435785
18	1	0	-0.004251	2.930046	-1.299318
19	1	0	1.018378	1.511357	-1.663402
20	1	0	1.310571	2.432923	-0.176605
21	1	0	-1.701495	1.185317	1.493168
22	6	0	2.196775	-0.439834	0.168116
23	8	0	2.147379	0.542882	0.887817
24	8	0	2.962912	-1.324133	-0.156346

TMG-$\mathbf{TS_{2/3}}$

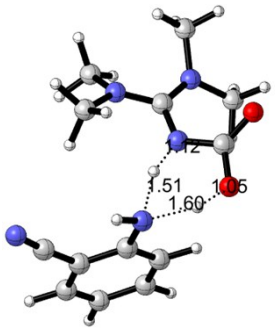
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.534520	-0.795913	0.060163
2	6	0	-0.350200	-0.147064	-0.130882
3	7	0	-0.412056	1.219206	-0.172736
4	7	0	0.730497	-0.871857	-0.330374
5	6	0	-1.511705	-2.222775	0.342160
6	6	0	-2.792321	-0.296242	-0.472460
7	6	0	-1.251888	1.971897	0.747176
8	6	0	0.633309	2.003971	-0.801659
9	1	0	3.361170	-0.731533	-1.102255
10	1	0	-0.641632	-2.464490	0.949974
11	1	0	-1.461258	-2.807884	-0.584992
12	1	0	-2.425687	-2.481732	0.884875
13	1	0	-2.633218	0.648007	-0.993698
14	1	0	-3.532500	-0.147576	0.322748
15	1	0	-3.194876	-1.024056	-1.187641
16	1	0	-0.609667	2.564604	1.410086
17	1	0	-1.922455	2.650790	0.205541
18	1	0	0.168613	2.875817	-1.274938
19	1	0	1.122327	1.408833	-1.575729
20	1	0	1.383005	2.331582	-0.072762
21	1	0	-1.844747	1.293454	1.360389
22	6	0	1.925848	-0.440812	0.171033
23	8	0	2.988776	-1.173258	-0.326104

24	8	0	2.114377	0.399544	1.029457

TMG-**$TS_{2/3}$'**

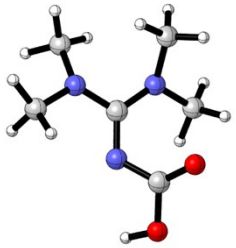


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.071302	-0.262476	-0.855594
2	7	0	-1.520753	1.757576	0.035797
3	6	0	-1.884285	0.459129	0.084955
4	7	0	-2.924510	0.093461	0.855636
5	7	0	-1.156733	-0.420999	-0.607450
6	6	0	-0.629763	2.244839	-1.017100
7	6	0	-1.674295	2.647022	1.181582
8	6	0	-4.106764	0.932344	1.003023
9	6	0	-3.043394	-1.247221	1.417405
10	1	0	-0.804384	1.690078	-1.939361
11	1	0	0.423936	2.143381	-0.729820
12	1	0	-0.852236	3.300672	-1.189696
13	1	0	-1.986573	2.079297	2.058452
14	1	0	-2.404117	3.438630	0.979563
15	1	0	-0.704749	3.108780	1.393212
16	1	0	-4.982358	0.341820	0.715056
17	1	0	-4.231751	1.270153	2.038192
18	1	0	-3.380706	-1.145221	2.453961
19	1	0	-2.069661	-1.738407	1.407700
20	1	0	-3.751487	-1.848631	0.842403
21	1	0	-4.040284	1.797091	0.342694
22	6	0	-1.658460	-1.581154	-1.264442
23	8	0	-0.691253	-2.269260	-1.824152
24	8	0	-2.835468	-1.856811	-1.307641
25	1	0	0.231688	-1.779819	-1.718271
26	7	0	1.295351	-0.641323	-1.359791
27	6	0	2.132014	-0.653987	-0.281664
28	6	0	1.956071	-1.622058	0.739917
29	6	0	2.768945	-1.649412	1.859083
30	6	0	3.169502	0.297632	-0.068692
31	6	0	3.994959	0.253154	1.065216

32	6	0	3.804369	-0.717463	2.034124
33	1	0	1.182181	-2.373826	0.601961
34	1	0	2.609202	-2.419531	2.609610
35	6	0	3.314583	1.349082	-1.030361
36	1	0	4.778576	0.998012	1.171345
37	1	0	4.443505	-0.755841	2.909545
38	1	0	1.622305	-0.014745	-2.094342
39	7	0	3.355371	2.198099	-1.821414

TMG-**3**

Standard orientation:

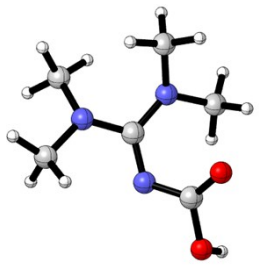


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.550081	-0.767607	0.066373
2	6	0	-0.346007	-0.150144	-0.118643
3	7	0	-0.372615	1.215418	-0.170751
4	7	0	0.719712	-0.899253	-0.291032
5	6	0	-1.571522	-2.186077	0.381680
6	6	0	-2.785535	-0.244274	-0.494293
7	6	0	-1.202616	1.996242	0.733860
8	6	0	0.685333	1.973456	-0.815377
9	1	0	2.595530	-1.752193	-1.014137
10	1	0	-0.716335	-2.436179	1.007432
11	1	0	-1.529601	-2.797398	-0.529423
12	1	0	-2.498558	-2.407024	0.919302
13	1	0	-2.593741	0.690392	-1.021786
14	1	0	-3.534934	-0.068658	0.286729
15	1	0	-3.194615	-0.969042	-1.209174
16	1	0	-0.552884	2.586267	1.391645
17	1	0	-1.857148	2.680131	0.178903
18	1	0	0.229562	2.834599	-1.316470
19	1	0	1.179273	1.353514	-1.566144
20	1	0	1.432041	2.315040	-0.090773
21	1	0	-1.812111	1.337876	1.352874
22	6	0	1.936237	-0.450706	0.180208
23	8	0	2.972721	-1.112956	-0.389114

24	8	0	2.149662	0.383180	1.035899

TMG-**TS$_{3/4}$**

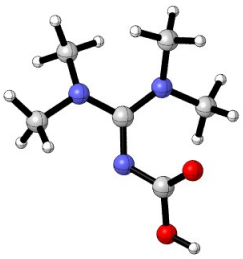
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.534520	-0.795913	0.060163
2	6	0	-0.350200	-0.147064	-0.130882
3	7	0	-0.412056	1.219206	-0.172736
4	7	0	0.730497	-0.871857	-0.330374
5	6	0	-1.511705	-2.222775	0.342160
6	6	0	-2.792321	-0.296242	-0.472460
7	6	0	-1.251888	1.971897	0.747176
8	6	0	0.633309	2.003971	-0.801659
9	1	0	3.361170	-0.731533	-1.102255
10	1	0	-0.641632	-2.464490	0.949974
11	1	0	-1.461258	-2.807884	-0.584992
12	1	0	-2.425687	-2.481732	0.884875
13	1	0	-2.633218	0.648007	-0.993698
14	1	0	-3.532500	-0.147576	0.322748
15	1	0	-3.194876	-1.024056	-1.187641
16	1	0	-0.609667	2.564604	1.410086
17	1	0	-1.922455	2.650790	0.205541
18	1	0	0.168613	2.875817	-1.274938
19	1	0	1.122327	1.408833	-1.575729
20	1	0	1.383005	2.331582	-0.072762
21	1	0	-1.844747	1.293454	1.360389
22	6	0	1.925848	-0.440812	0.171033
23	8	0	2.988776	-1.173258	-0.326104
24	8	0	2.114377	0.399544	1.029457

TMG-**4**

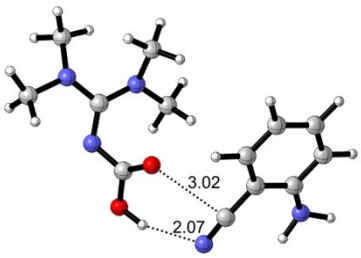
Standard orientation:



Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.571956	-0.751895	0.074583
2	6	0	-0.359933	-0.151255	-0.119278
3	7	0	-0.368737	1.217333	-0.166618
4	7	0	0.689290	-0.913074	-0.312914
5	6	0	-1.601293	-2.177764	0.357469
6	6	0	-2.798923	-0.216879	-0.494666
7	6	0	-1.185236	2.004612	0.744086
8	6	0	0.710458	1.957411	-0.794626
9	1	0	3.730268	-0.829678	-0.072626
10	1	0	-0.757049	-2.444609	0.991107
11	1	0	-1.542635	-2.767563	-0.566541
12	1	0	-2.537735	-2.407095	0.874723
13	1	0	-2.600395	0.728327	-1.000275
14	1	0	-3.559039	-0.057615	0.279316
15	1	0	-3.197702	-0.926465	-1.230592
16	1	0	-0.527140	2.575039	1.411415
17	1	0	-1.824259	2.707569	0.194796
18	1	0	0.281463	2.838857	-1.283717
19	1	0	1.190782	1.335698	-1.553190
20	1	0	1.461724	2.270257	-0.060427
21	1	0	-1.810150	1.351736	1.353470
22	6	0	1.903315	-0.498065	0.148113
23	8	0	2.912479	-1.125087	-0.504236
24	8	0	2.142691	0.281416	1.060560

TMG-**5**



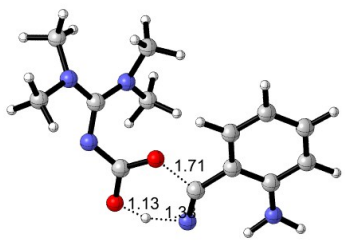
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.052607	-0.415742	-0.118045
2	6	0	-2.782754	-0.005344	0.184456
3	7	0	-1.945643	-0.972007	0.686859
4	7	0	-2.481968	1.258243	0.044352
5	6	0	-4.915736	0.503911	-0.840664

6	6	0	-4.752576	-1.406076	0.684517
7	6	0	-1.905490	-2.306628	0.112493
8	6	0	-0.768521	-0.620182	1.459588
9	1	0	-4.337803	1.034769	-1.595919
10	1	0	-5.364208	1.243450	-0.164357
11	1	0	-5.709258	-0.074569	-1.323135
12	1	0	-4.079635	-1.833032	1.427992
13	1	0	-5.150525	-2.210961	0.055147
14	1	0	-5.591286	-0.928690	1.207954
15	1	0	-0.941502	-2.451776	-0.393374
16	1	0	-2.011204	-3.073311	0.890558
17	1	0	-0.632447	-1.375461	2.241515
18	1	0	-0.913935	0.352543	1.934398
19	1	0	0.130870	-0.581154	0.832530
20	1	0	-2.702901	-2.427510	-0.621141
21	6	0	-1.202638	1.595864	-0.301715
22	8	0	-0.426171	0.926250	-0.976795
23	8	0	-0.877537	2.820912	0.139830
24	1	0	0.045680	2.996313	-0.127501
25	6	0	4.001819	-0.067330	0.415610
26	6	0	4.467649	-1.387195	0.299309
27	6	0	3.829403	-2.288734	-0.538593
28	6	0	2.706038	-1.915222	-1.285843
29	6	0	2.870226	0.300287	-0.344731
30	6	0	2.227473	-0.617498	-1.187424
31	6	0	2.406743	1.651914	-0.240385
32	7	0	2.106231	2.764365	-0.110404
33	1	0	2.216294	-2.629922	-1.938688
34	1	0	4.213891	-3.302341	-0.611430
35	1	0	5.333200	-1.694230	0.880482
36	1	0	1.348435	-0.287069	-1.731526
37	7	0	4.594593	0.822552	1.285579
38	1	0	4.392889	1.806885	1.158457
39	1	0	5.549037	0.630284	1.555667

TMG-**$TS_{5/6}$**

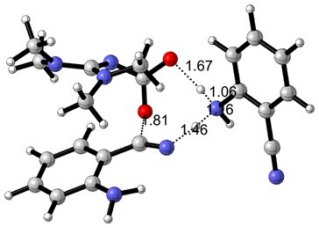
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.671515	-0.472099	-0.467854
2	6	0	-2.572759	0.062782	0.130825
3	7	0	-1.936657	-0.715447	1.055945
4	7	0	-2.247369	1.307142	-0.158200
5	6	0	-4.245369	0.217883	-1.614006
6	6	0	-4.586151	-1.359139	0.236288
7	6	0	-1.769311	-2.149245	0.866361
8	6	0	-1.055174	-0.139639	2.058353
9	1	0	-3.451502	0.655188	-2.217344
10	1	0	-4.921975	1.019819	-1.292863
11	1	0	-4.802194	-0.510373	-2.210536
12	1	0	-4.238406	-1.529660	1.255310
13	1	0	-4.683225	-2.322203	-0.278048
14	1	0	-5.575767	-0.888828	0.282825
15	1	0	-0.696937	-2.374685	0.809618
16	1	0	-2.202289	-2.715286	1.700463
17	1	0	-1.204911	-0.679726	2.999253
18	1	0	-1.304157	0.911508	2.216267
19	1	0	-0.003109	-0.223421	1.759578
20	1	0	-2.239570	-2.464905	-0.065331
21	6	0	-0.950067	1.668663	-0.193941
22	8	0	-0.038135	0.791278	-0.464138
23	8	0	-0.652625	2.902088	-0.005694
24	1	0	0.473908	2.939886	0.000229
25	6	0	3.702368	0.087726	0.085213
26	6	0	4.466867	-1.091910	-0.012344
27	6	0	3.914050	-2.266946	-0.491119
28	6	0	2.574951	-2.312744	-0.892492
29	6	0	2.341708	0.037431	-0.314607
30	6	0	1.804492	-1.162568	-0.799931
31	6	0	1.577719	1.282741	-0.215049
32	7	0	1.764586	2.455940	0.010356
33	1	0	2.144728	-3.231105	-1.278773
34	1	0	4.533050	-3.157878	-0.554082
35	1	0	5.507271	-1.064743	0.302742
36	1	0	0.768840	-1.170540	-1.117786
37	7	0	4.259697	1.228410	0.601262

38	1	0	3.754318	2.098928	0.464586
39	1	0	5.266886	1.283252	0.630690

TMG-**TS$_{5/6}$'**

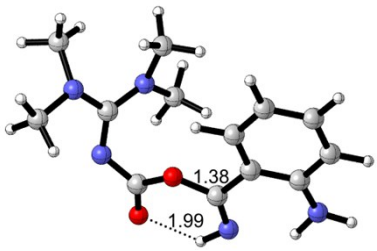


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.138688	-2.074033	0.198082
2	6	0	1.808740	-1.758958	0.028522
3	7	0	1.155814	-1.307833	1.158734
4	7	0	1.255142	-1.921579	-1.126810
5	6	0	3.938622	-2.320863	-0.985729
6	6	0	3.597405	-2.779196	1.383483
7	6	0	1.792582	-0.463406	2.154009
8	6	0	-0.262190	-1.547901	1.342132
9	1	0	3.637992	-1.641578	-1.782272
10	1	0	3.815260	-3.351501	-1.348022
11	1	0	4.990754	-2.148946	-0.736343
12	1	0	2.812243	-2.805396	2.138867
13	1	0	4.483575	-2.291455	1.806837
14	1	0	3.860481	-3.814704	1.125958
15	1	0	1.212928	0.460966	2.275980
16	1	0	1.851529	-0.968160	3.129120
17	1	0	-0.438891	-1.835480	2.386352
18	1	0	-0.582204	-2.362353	0.689682
19	1	0	-0.864558	-0.653517	1.128354
20	1	0	2.798906	-0.196177	1.824346
21	6	0	0.149747	-1.206489	-1.550275
22	8	0	0.287077	0.068945	-1.781907
23	8	0	-0.929379	-1.784680	-1.807168
24	6	0	2.198841	2.540090	0.664487
25	6	0	3.559506	2.870082	0.798481
26	6	0	4.516141	2.311664	-0.034550
27	6	0	4.149514	1.407087	-1.035268
28	6	0	1.833282	1.611027	-0.343319
29	6	0	2.812626	1.068562	-1.182828

30	6	0	0.417416	1.274131	-0.437524
31	7	0	-0.648843	1.562681	0.027510
32	1	0	4.897130	0.978246	-1.694912
33	1	0	5.559072	2.587854	0.095920
34	1	0	3.852658	3.569296	1.578086
35	1	0	2.486209	0.378681	-1.951916
36	7	0	1.274701	3.057493	1.546013
37	1	0	0.298249	2.986100	1.276262
38	1	0	1.533352	3.914165	2.015110
39	1	0	-1.739127	0.909042	-0.683810
40	1	0	-1.961215	-0.477884	-1.728330
41	7	0	-2.524910	0.317288	-1.302840
42	1	0	-2.862623	0.946774	-2.035207
43	6	0	-3.575650	-0.193479	-0.463331
44	6	0	-3.574335	-1.537922	-0.104247
45	6	0	-4.559530	0.669246	0.037866
46	6	0	-4.558564	-2.015262	0.758507
47	6	0	-5.542796	-1.163226	1.259859
48	6	0	-5.548095	0.178594	0.897605
49	6	0	-4.551285	2.051504	-0.359401
50	7	0	-4.527653	3.153316	-0.714400
51	1	0	-2.804525	-2.189617	-0.510628
52	1	0	-4.557515	-3.065005	1.035687
53	1	0	-6.307059	-1.543997	1.929402
54	1	0	-6.306635	0.857490	1.273178

TMG-**6**



Standard orientation:

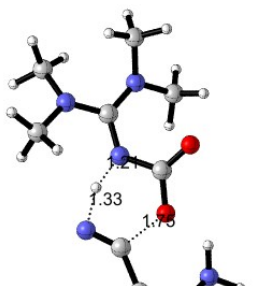
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.371842	-0.647267	-0.515728
2	6	0	-2.395329	0.077808	0.109675
3	7	0	-1.736832	-0.547930	1.132395
4	7	0	-2.210487	1.321648	-0.261726
5	6	0	-3.915716	-0.130431	-1.762447
6	6	0	-4.278814	-1.508035	0.231794

7	6	0	-1.480515	-1.980940	1.139726
8	6	0	-0.998906	0.202190	2.134542
9	1	0	-3.115561	0.297201	-2.365072
10	1	0	-4.667407	0.647749	-1.578178
11	1	0	-4.377635	-0.961056	-2.303855
12	1	0	-4.003838	-1.525349	1.286445
13	1	0	-4.269429	-2.532107	-0.159212
14	1	0	-5.299211	-1.113734	0.150456
15	1	0	-0.402333	-2.147384	1.248674
16	1	0	-1.996316	-2.477835	1.971318
17	1	0	-1.154470	-0.273764	3.108612
18	1	0	-1.369535	1.227318	2.188125
19	1	0	0.077484	0.210830	1.919154
20	1	0	-1.806278	-2.425468	0.198233
21	6	0	-0.997139	1.925863	-0.188543
22	8	0	0.025802	1.034961	-0.494563
23	1	0	1.195427	3.161230	-0.041757
24	6	0	3.517430	-0.024871	-0.014472
25	6	0	4.175122	-1.273779	-0.079275
26	6	0	3.503145	-2.429535	-0.428020
27	6	0	2.137186	-2.391375	-0.732184
28	6	0	2.129296	0.016555	-0.317647
29	6	0	1.476230	-1.175317	-0.674381
30	6	0	1.368806	1.285369	-0.268218
31	7	0	1.894576	2.418763	-0.042134
32	1	0	1.605519	-3.293420	-1.017823
33	1	0	4.046549	-3.369842	-0.466696
34	1	0	5.235440	-1.309778	0.159858
35	7	0	4.220295	1.078738	0.369359
36	8	0	-0.792938	3.099041	0.028993
37	1	0	0.421094	-1.124780	-0.921540
38	1	0	3.776123	1.986571	0.272853
39	1	0	5.226719	1.022929	0.396519

TMG-**$TS_{2/6}$'**

Standard orientation:

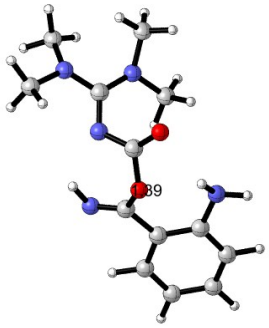
Center	Atomic	Atomic	Coordinates (Angstroms)



Number	Number	Type	X	Y	Z
1	7	0	3.232433	1.386258	0.001455
2	6	0	2.644109	0.165287	-0.045877
3	7	0	3.432990	-0.920494	-0.204640
4	7	0	1.321319	0.108600	0.015775
5	6	0	2.470353	2.540210	0.468441
6	6	0	4.435018	1.699612	-0.757624
7	6	0	4.732595	-1.027838	0.442726
8	6	0	2.924628	-2.164066	-0.766087
9	1	0	0.541544	0.951672	-0.380406
10	1	0	1.772866	2.232097	1.247610
11	1	0	1.902563	3.002178	-0.348205
12	1	0	3.172986	3.269731	0.879854
13	1	0	4.726159	0.845976	-1.370241
14	1	0	5.265824	1.970788	-0.096184
15	1	0	4.224398	2.547133	-1.419245
16	1	0	4.718165	-1.898679	1.107273
17	1	0	5.533534	-1.158540	-0.294474
18	1	0	3.696002	-2.573942	-1.426642
19	1	0	2.027005	-1.962232	-1.351987
20	1	0	2.679019	-2.878460	0.024313
21	1	0	4.932039	-0.138925	1.041075
22	6	0	0.588402	-0.911647	0.676052
23	8	0	1.126122	-1.772325	1.349811
24	8	0	-0.698542	-0.786579	0.506086
25	7	0	-0.651493	1.477460	-0.652787
26	6	0	-1.400714	0.624732	-0.249976
27	6	0	-2.843682	0.393917	-0.095489
28	6	0	-3.494624	-0.840056	-0.312924
29	6	0	-3.597971	1.536502	0.203975
30	6	0	-4.980653	1.489455	0.308088
31	6	0	-4.897517	-0.867310	-0.212516
32	6	0	-5.627382	0.270602	0.093186
33	7	0	-2.815193	-1.986298	-0.696002
34	1	0	-3.356876	-2.835554	-0.598432
35	1	0	-1.884170	-2.066340	-0.299638
36	1	0	-3.063549	2.470700	0.349289
37	1	0	-5.544394	2.384535	0.549176
38	1	0	-6.709629	0.205073	0.166303

39	1	0	-5.409902	-1.811062	-0.385061

TMG-**6'**

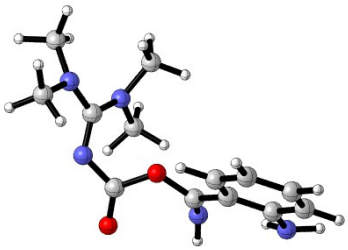


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.706559	-0.770662	-0.130417
2	6	0	-2.530558	-0.091300	-0.056114
3	7	0	-2.479715	1.130332	-0.660194
4	7	0	-1.498242	-0.678055	0.517803
5	6	0	-3.889835	-1.950271	0.700875
6	6	0	-4.579440	-0.691177	-1.292439
7	6	0	-3.598608	2.059684	-0.593127
8	6	0	-1.208555	1.743975	-1.014444
9	1	0	-0.131970	-2.296368	0.004131
10	1	0	-3.393612	-1.806280	1.659419
11	1	0	-3.474359	-2.844580	0.218711
12	1	0	-4.961988	-2.095056	0.862302
13	1	0	-4.154785	-0.017888	-2.037145
14	1	0	-5.579966	-0.338871	-1.015651
15	1	0	-4.673587	-1.688128	-1.739150
16	1	0	-3.287051	2.946974	-0.029104
17	1	0	-3.914783	2.371953	-1.595681
18	1	0	-1.357034	2.329302	-1.927324
19	1	0	-0.460761	0.973277	-1.216063
20	1	0	-0.838672	2.396804	-0.215417
21	1	0	-4.441127	1.602333	-0.074406
22	6	0	-0.628052	0.093374	1.218806
23	8	0	-0.856261	1.105642	1.851485
24	8	0	0.670551	-0.371355	1.278388
25	7	0	0.808035	-2.094728	-0.338799
26	6	0	1.290122	-1.092386	0.259377
27	6	0	2.653010	-0.572040	-0.011220
28	6	0	3.025462	0.780151	0.172191

29	6	0	3.587890	-1.483864	-0.519910
30	6	0	4.879764	-1.101922	-0.846790
31	6	0	4.339148	1.151396	-0.170575
32	6	0	5.249496	0.233248	-0.668549
33	7	0	2.139253	1.777376	0.576295
34	1	0	2.598033	2.645461	0.823330
35	1	0	1.441063	1.510962	1.262192
36	1	0	3.259415	-2.510069	-0.652876
37	1	0	5.588055	-1.828154	-1.231815
38	1	0	6.255817	0.560724	-0.915403
39	1	0	4.634530	2.190269	-0.040326

TMG-**TS$_{6/7}$**



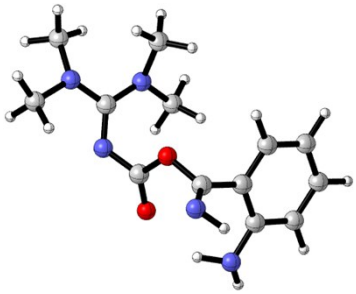
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.438914	1.063126	-0.013867
2	6	0	2.576739	0.006218	-0.096555
3	7	0	2.342344	-0.672192	1.074744
4	7	0	2.104593	-0.327346	-1.267897
5	6	0	3.569389	1.940365	-1.165402
6	6	0	4.579038	1.062964	0.889162
7	6	0	2.085203	0.038478	2.316511
8	6	0	1.850841	-2.040618	1.044886
9	1	0	2.597094	2.073690	-1.637651
10	1	0	4.261180	1.522293	-1.908120
11	1	0	3.948498	2.907093	-0.821163
12	1	0	4.561253	0.173341	1.518542
13	1	0	4.576421	1.955174	1.526371
14	1	0	5.508106	1.057372	0.304882
15	1	0	1.026650	-0.071521	2.588385
16	1	0	2.700504	-0.363441	3.131159
17	1	0	2.269311	-2.571387	1.907297
18	1	0	2.190697	-2.533814	0.131874
19	1	0	0.756406	-2.094058	1.087295
20	1	0	2.299895	1.100672	2.196016

21	6	0	0.866031	-0.885778	-1.407018
22	8	0	-0.055644	-0.306941	-0.520399
23	1	0	-1.663240	-3.029090	-0.652110
24	6	0	-3.628939	-0.217447	0.348032
25	6	0	-4.567524	0.816527	0.541406
26	6	0	-4.255565	2.133551	0.260782
27	6	0	-2.986668	2.474286	-0.221506
28	6	0	-2.338383	0.121667	-0.132945
29	6	0	-2.049285	1.472133	-0.403578
30	6	0	-1.300218	-0.916346	-0.342872
31	7	0	-1.405823	-2.152700	-0.249064
32	1	0	-2.739179	3.505785	-0.449475
33	1	0	-5.007129	2.903190	0.414134
34	1	0	-5.558057	0.554651	0.906190
35	7	0	-4.016365	-1.513874	0.601913
36	8	0	0.523522	-1.667896	-2.254612
37	1	0	-1.059162	1.716622	-0.770366
38	1	0	-3.269751	-2.192943	0.681440
39	1	0	-4.792117	-1.630036	1.239179

TMG-7

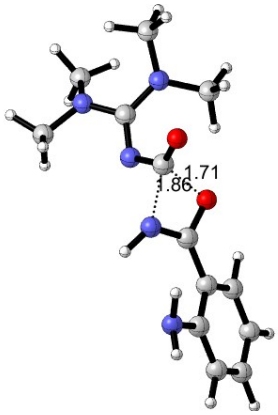
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.763712	-0.131310	0.082305
2	6	0	-2.469717	-0.007806	-0.321867
3	7	0	-1.962104	1.266094	-0.373413
4	7	0	-1.821732	-1.075128	-0.714095
5	6	0	-4.279950	-1.459505	0.373530
6	6	0	-4.771163	0.878181	-0.201680
7	6	0	-2.207774	2.224222	0.691669
8	6	0	-0.808675	1.557129	-1.209558
9	1	0	-3.489264	-2.073749	0.801909
10	1	0	-4.648766	-1.948219	-0.537394
11	1	0	-5.100879	-1.362609	1.090110
12	1	0	-4.324671	1.715314	-0.738873

13	1	0	-5.233938	1.247400	0.721273
14	1	0	-5.555492	0.439140	-0.830537
15	1	0	-1.266876	2.428278	1.219229
16	1	0	-2.596413	3.168922	0.291847
17	1	0	-0.894970	2.589369	-1.564851
18	1	0	-0.800278	0.887652	-2.071671
19	1	0	0.137606	1.452016	-0.664200
20	1	0	-2.920543	1.816504	1.408807
21	6	0	-0.496316	-1.224851	-0.477578
22	8	0	-0.106756	-0.719411	0.755167
23	6	0	3.221556	-0.516553	-0.334195
24	6	0	4.191787	0.404417	-0.762590
25	6	0	4.169316	1.722644	-0.327503
26	6	0	3.172592	2.170322	0.542170
27	6	0	2.224971	-0.064700	0.553245
28	6	0	2.204855	1.267902	0.970553
29	6	0	1.211822	-1.016201	1.091503
30	7	0	1.406191	-2.015091	1.832500
31	1	0	3.154968	3.200652	0.882258
32	1	0	4.934589	2.410176	-0.677054
33	1	0	4.966104	0.070324	-1.449221
34	7	0	3.264502	-1.847881	-0.727026
35	8	0	0.303637	-1.808988	-1.180774
36	1	0	1.419794	1.587314	1.653138
37	1	0	2.341305	-2.263213	-0.848024
38	1	0	3.853819	-2.018173	-1.532879
39	1	0	2.407021	-2.107902	2.022889

TMG-**TS$_{7/8}$**



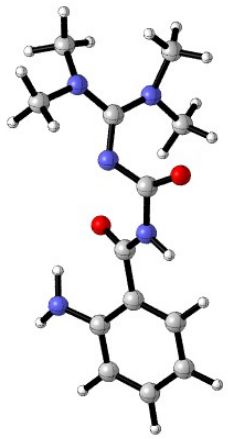
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.489496	1.086628	0.787228
2	6	0	-2.644639	0.189083	0.175188
3	7	0	-3.205673	-1.019268	-0.146474
4	7	0	-1.403284	0.549866	-0.010427

5	6	0	-3.037400	2.458514	0.936684
6	6	0	-4.439417	0.654908	1.800875
7	6	0	-4.557629	-1.117943	-0.668370
8	6	0	-2.403703	-2.219981	-0.304511
9	1	0	-2.516918	2.773612	0.033116
10	1	0	-2.350609	2.565973	1.787467
11	1	0	-3.913860	3.093804	1.098412
12	1	0	-4.506407	-0.432841	1.821341
13	1	0	-5.434718	1.070742	1.604206
14	1	0	-4.109660	0.999062	2.790793
15	1	0	-4.520480	-1.517156	-1.689829
16	1	0	-5.171858	-1.789860	-0.054420
17	1	0	-2.956772	-3.059842	0.132467
18	1	0	-1.455853	-2.107293	0.223190
19	1	0	-2.191970	-2.427733	-1.359278
20	1	0	-5.023117	-0.132327	-0.695999
21	6	0	-0.707426	-0.018794	-1.052331
22	8	0	-1.064877	-0.410901	-2.124989
23	6	0	3.837006	0.593771	-0.399560
24	6	0	5.086033	0.440679	0.221182
25	6	0	5.252778	-0.441302	1.279417
26	6	0	4.182748	-1.210207	1.743874
27	6	0	2.751127	-0.161025	0.088566
28	6	0	2.943062	-1.066989	1.138106
29	6	0	1.394390	-0.021436	-0.468207
30	1	0	4.318112	-1.909249	2.562299
31	1	0	6.232340	-0.538088	1.739362
32	1	0	5.930281	1.021630	-0.142698
33	7	0	3.684057	1.503885	-1.445492
34	1	0	4.558946	1.787137	-1.870350
35	1	0	2.999441	1.237919	-2.146721
36	7	0	0.860263	0.978837	-1.099350
37	1	0	1.264704	1.911499	-1.075280
38	8	0	0.527261	-0.973578	-0.346408
39	1	0	2.086683	-1.646452	1.469215

TMG-**8**

Standard orientation:

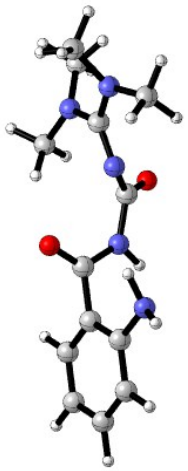


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.684763	1.013835	0.430674
2	6	0	2.705450	0.120667	0.101177
3	7	0	3.029350	-0.811999	-0.854310
4	7	0	1.521787	0.247201	0.636918
5	6	0	3.459833	1.888683	1.569308
6	6	0	4.629003	1.519649	-0.553371
7	6	0	4.308460	-1.504158	-0.821700
8	6	0	1.980888	-1.515616	-1.571962
9	1	0	-1.120744	-1.430111	1.289228
10	1	0	2.950810	1.339614	2.360296
11	1	0	2.842492	2.752869	1.291058
12	1	0	4.430313	2.239047	1.932985
13	1	0	4.497091	1.002389	-1.503657
14	1	0	5.661876	1.386832	-0.210327
15	1	0	4.451646	2.590902	-0.714104
16	1	0	4.148755	-2.548236	-0.521593
17	1	0	4.784537	-1.489382	-1.809939
18	1	0	2.354807	-1.758612	-2.572040
19	1	0	1.108508	-0.864554	-1.673481
20	1	0	1.690896	-2.442476	-1.059554
21	1	0	4.974450	-1.037005	-0.096013
22	6	0	0.791086	-0.865862	0.909039
23	8	0	1.208854	-1.931315	1.345690
24	8	0	-0.764179	0.919851	-0.803824
25	6	0	-3.397490	-1.273379	0.277076
26	6	0	-4.774960	-1.433339	0.307832
27	6	0	-5.584204	-0.324620	0.044878
28	6	0	-5.019829	0.901070	-0.262855
29	6	0	-2.799595	-0.040169	-0.017153
30	6	0	-3.622953	1.071854	-0.320935
31	6	0	-1.311909	0.115280	-0.063171
32	7	0	-3.100881	2.314638	-0.598151
33	7	0	-0.609855	-0.721929	0.779363
34	1	0	-2.151836	2.329479	-0.952712
35	1	0	-3.733787	2.981096	-1.016849
36	1	0	-5.656498	1.757521	-0.472275

37	1	0	-6.666070	-0.421574	0.069990
38	1	0	-5.211395	-2.402478	0.524403
39	1	0	-2.772090	-2.146198	0.449233

TMG-**TS$_{8/9}$**

Standard orientation:

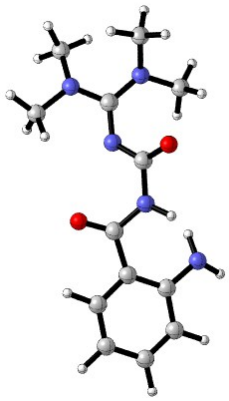


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.498832	1.216364	-0.118886
2	6	0	2.628972	0.170720	0.012058
3	7	0	3.125637	-1.072798	-0.282593
4	7	0	1.384480	0.414865	0.328327
5	6	0	3.092044	2.517098	0.384451
6	6	0	4.506340	1.252408	-1.167839
7	6	0	4.448589	-1.481064	0.162739
8	6	0	2.226499	-2.169206	-0.598151
9	1	0	-1.246614	-0.880953	1.596961
10	1	0	2.538507	2.394580	1.314615
11	1	0	2.452923	3.041917	-0.338173
12	1	0	3.991272	3.112240	0.569796
13	1	0	4.507457	0.314449	-1.723175
14	1	0	5.504748	1.424324	-0.748580
15	1	0	4.277651	2.067582	-1.866239
16	1	0	4.346870	-2.248169	0.941159
17	1	0	5.030342	-1.897310	-0.669048
18	1	0	2.731541	-2.830736	-1.309884
19	1	0	1.321369	-1.775774	-1.068316
20	1	0	1.957099	-2.741612	0.298828
21	1	0	4.984127	-0.631081	0.586075
22	6	0	0.703582	-0.481935	1.095027
23	8	0	1.137663	-1.132581	2.035059
24	8	0	-0.738547	-0.150474	-1.434303
25	6	0	-3.618449	-1.338103	-0.469366
26	6	0	-5.004917	-1.244448	-0.375575
27	6	0	-5.578307	-0.010627	-0.069162
28	6	0	-4.784689	1.112339	0.135573

29	6	0	-2.815245	-0.221135	-0.254818
30	6	0	-3.389214	1.026898	0.041778
31	6	0	-1.317806	-0.304645	-0.376460
32	7	0	-2.580851	2.133091	0.295640
33	7	0	-0.683573	-0.542417	0.825303
34	1	0	-1.670841	2.124890	-0.153250
35	1	0	-3.040587	3.028240	0.187894
36	1	0	-5.243243	2.070010	0.370972
37	1	0	-6.658053	0.082634	0.007164
38	1	0	-5.626679	-2.117818	-0.542936
39	1	0	-3.146874	-2.286514	-0.715980

TMG-**9**

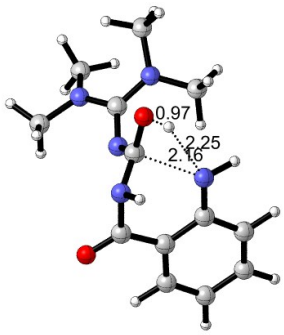
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.434863	1.324847	-0.150720
2	6	0	2.744672	0.151415	-0.105303
3	7	0	3.485309	-0.996203	-0.142688
4	7	0	1.429281	0.223465	-0.099849
5	6	0	2.711557	2.567844	0.085564
6	6	0	4.685594	1.469426	-0.877816
7	6	0	4.730869	-1.130113	0.595800
8	6	0	2.912690	-2.250724	-0.594358
9	1	0	-1.207438	-1.299028	0.880268
10	1	0	1.909122	2.399696	0.801322
11	1	0	2.261396	2.940067	-0.843086
12	1	0	3.417504	3.308306	0.473639
13	1	0	4.951059	0.530543	-1.365067
14	1	0	5.504040	1.774527	-0.214634
15	1	0	4.562120	2.238237	-1.649862
16	1	0	4.609385	-1.912564	1.354632
17	1	0	5.560914	-1.407674	-0.066247
18	1	0	3.668995	-2.779691	-1.185617
19	1	0	2.047447	-2.048244	-1.228175
20	1	0	2.594460	-2.870323	0.250044

21	1	0	4.971934	-0.195360	1.102291
22	6	0	0.701362	-0.661064	0.623916
23	8	0	1.086237	-1.520683	1.411688
24	8	0	-0.964581	1.686560	-0.086796
25	6	0	-3.723877	1.458545	0.301948
26	6	0	-5.108630	1.382770	0.290680
27	6	0	-5.712854	0.170723	-0.049719
28	6	0	-4.938187	-0.930266	-0.382246
29	6	0	-2.922837	0.350727	-0.000590
30	6	0	-3.535431	-0.864017	-0.371175
31	6	0	-1.437416	0.582507	0.084490
32	7	0	-2.805840	-2.016160	-0.684844
33	7	0	-0.697925	-0.546673	0.425149
34	1	0	-1.907095	-1.856548	-1.125616
35	1	0	-3.345705	-2.713882	-1.182216
36	1	0	-5.415753	-1.866221	-0.663690
37	1	0	-6.795729	0.083765	-0.066533
38	1	0	-5.709391	2.250550	0.542222
39	1	0	-3.215396	2.385251	0.550704

TMG-**TS$_{9/10}$**

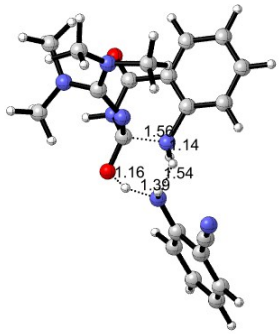


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.842166	0.996635	-0.783186
2	6	0	2.002049	0.081827	-0.243053
3	7	0	2.409010	-1.212964	-0.241896
4	7	0	0.829494	0.536270	0.187948
5	6	0	2.577174	2.418111	-0.583186
6	6	0	3.749176	0.681106	-1.877393
7	6	0	3.787702	-1.592052	0.025922
8	6	0	1.448642	-2.300735	-0.210048
9	1	0	2.133203	2.580602	0.397100
10	1	0	1.883484	2.795407	-1.343136
11	1	0	3.527663	2.954124	-0.654600
12	1	0	3.565876	-0.331057	-2.239438

13	1	0	4.798691	0.774377	-1.574844
14	1	0	3.561285	1.381971	-2.697873
15	1	0	3.800577	-2.253879	0.899815
16	1	0	4.233607	-2.124182	-0.823118
17	1	0	1.810436	-3.096029	-0.870916
18	1	0	0.480367	-1.944506	-0.559795
19	1	0	1.336095	-2.697626	0.806023
20	1	0	4.384751	-0.709387	0.255404
21	6	0	0.265479	0.142303	1.324061
22	8	0	0.972051	-0.582468	2.221673
23	8	0	-1.770556	2.709918	0.728656
24	6	0	-3.342578	0.975822	-0.866238
25	6	0	-4.106788	0.118379	-1.628691
26	6	0	-3.909132	-1.268560	-1.469903
27	6	0	-2.979474	-1.760414	-0.582134
28	6	0	-2.391515	0.503650	0.059801
29	6	0	-2.169314	-0.906035	0.233155
30	6	0	-1.650271	1.509767	0.814890
31	7	0	-1.240129	-1.393531	1.084389
32	7	0	-0.710609	0.971749	1.812106
33	1	0	-1.223218	0.525555	2.570768
34	1	0	-2.845591	-2.835807	-0.476521
35	1	0	-4.498895	-1.967108	-2.059628
36	1	0	-4.841892	0.498296	-2.330231
37	1	0	-3.456683	2.053174	-0.952788
38	1	0	0.311644	-1.124087	2.691430
39	1	0	-1.169790	-2.405576	0.961086

TMG-**TS$_{9/10}$'**



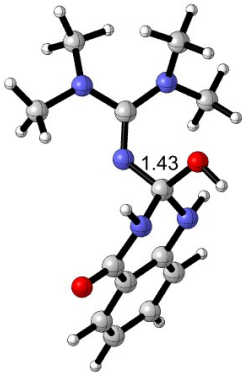
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.608918	-1.228015	1.711968
2	6	0	-2.076657	-1.325048	0.443431
3	7	0	-2.890062	-1.940110	-0.485320
4	7	0	-0.903230	-0.818633	0.233754

5	6	0	-1.967178	-0.327971	2.655335
6	6	0	-3.265558	-2.373179	2.325623
7	6	0	-4.335957	-1.811458	-0.462909
8	6	0	-2.361740	-2.797108	-1.527147
9	1	0	-1.739930	0.620361	2.165462
10	1	0	-1.032522	-0.748212	3.050465
11	1	0	-2.661510	-0.150302	3.482042
12	1	0	-3.472726	-3.138076	1.576818
13	1	0	-4.208143	-2.072237	2.797224
14	1	0	-2.614900	-2.812435	3.093911
15	1	0	-4.677956	-1.435330	-1.434886
16	1	0	-4.824706	-2.776854	-0.268677
17	1	0	-2.738356	-3.820584	-1.391658
18	1	0	-1.271428	-2.807484	-1.499219
19	1	0	-2.694426	-2.457610	-2.518716
20	1	0	-4.633408	-1.098393	0.306684
21	6	0	-0.431543	-0.408707	-1.048777
22	8	0	0.437415	-1.238984	-1.646997
23	8	0	-3.409795	1.211114	-2.130092
24	6	0	-2.651836	2.916859	0.031691
25	6	0	-2.180921	3.767820	1.030597
26	6	0	-0.857961	3.677236	1.460769
27	6	0	0.005629	2.735579	0.897320
28	6	0	-1.800816	1.973941	-0.536433
29	6	0	-0.474920	1.896839	-0.095991
30	6	0	-2.316897	1.057765	-1.611765
31	7	0	0.368765	0.887023	-0.694977
32	7	0	-1.433048	0.081306	-1.991819
33	1	0	-1.766310	-0.584846	-2.680009
34	1	0	1.034457	2.642805	1.233981
35	1	0	-0.493032	4.336432	2.242452
36	1	0	-2.847012	4.500813	1.474874
37	1	0	-3.676889	2.965406	-0.323610
38	1	0	1.215997	0.407945	-0.098209
39	7	0	2.165045	-0.793248	0.096971
40	1	0	2.060597	-1.188101	1.029923
41	6	0	3.465736	-0.498447	-0.232326
42	6	0	4.532257	-0.490634	0.702864
43	6	0	5.838028	-0.146409	0.325037
44	6	0	6.120482	0.205568	-0.984979

45	6	0	5.080170	0.201705	-1.924023
46	6	0	3.788326	-0.143335	-1.562636
47	1	0	6.620377	-0.159268	1.078614
48	1	0	7.130595	0.471155	-1.277486
49	1	0	2.998330	-0.182335	-2.309912
50	1	0	5.289011	0.460590	-2.958830
51	6	0	4.240992	-0.829408	2.065527
52	7	0	3.959557	-1.100692	3.157738
53	1	0	1.302190	-1.266232	-0.881469
54	1	0	0.776149	1.212680	-1.578502

TMG-**10**

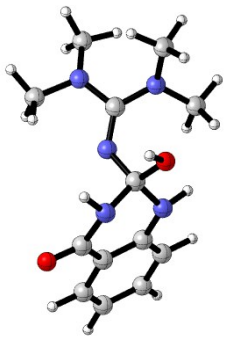


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.740617	1.136127	-0.945351
2	6	0	2.033654	0.141651	-0.307636
3	7	0	2.790807	-0.993941	-0.035552
4	7	0	0.780348	0.352280	-0.064999
5	6	0	2.119379	2.437570	-1.112484
6	6	0	3.817147	0.852881	-1.878350
7	6	0	4.000532	-0.884657	0.758287
8	6	0	2.194774	-2.309664	-0.064227
9	1	0	1.538925	2.687269	-0.224889
10	1	0	1.441868	2.452324	-1.976787
11	1	0	2.907642	3.181861	-1.261730
12	1	0	4.071848	-0.206069	-1.847308
13	1	0	4.707170	1.442698	-1.628232
14	1	0	3.509068	1.112292	-2.900611
15	1	0	3.801234	-1.173554	1.800530
16	1	0	4.782422	-1.539155	0.352908
17	1	0	2.956274	-3.026994	-0.393151
18	1	0	1.389761	-2.322342	-0.804782
19	1	0	1.812338	-2.628171	0.914554
20	1	0	4.360893	0.145330	0.744287
21	6	0	0.051610	-0.224419	1.020335

22	8	0	0.916317	-0.740531	2.001664
23	8	0	-2.297540	2.452269	1.335344
24	6	0	-3.757632	0.780858	-0.486881
25	6	0	-4.419922	-0.102322	-1.328624
26	6	0	-3.891801	-1.383179	-1.524339
27	6	0	-2.718790	-1.776020	-0.893638
28	6	0	-2.579209	0.397233	0.153654
29	6	0	-2.047181	-0.883997	-0.047815
30	6	0	-1.886652	1.334951	1.068412
31	7	0	-0.892193	-1.267142	0.633409
32	7	0	-0.748112	0.819893	1.659122
33	1	0	-0.171797	1.539539	2.087243
34	1	0	-2.315592	-2.773817	-1.050292
35	1	0	-4.400185	-2.083965	-2.181005
36	1	0	-5.336212	0.194665	-1.828280
37	1	0	-4.132754	1.783171	-0.301040
38	1	0	0.345130	-1.041507	2.727349
39	1	0	-0.413965	-2.053312	0.208606

TMG-**TS$_{10/11}$**



Standard orientation:

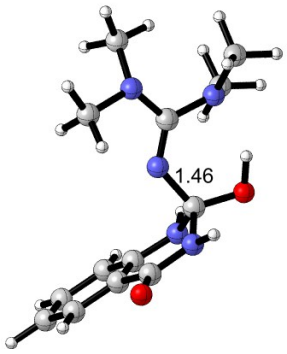
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.754029	1.097616	-0.968295
2	6	0	2.020774	0.144849	-0.284736
3	7	0	2.744310	-1.008282	0.000500
4	7	0	0.787794	0.416108	-0.008804
5	6	0	2.154809	2.404560	-1.173935
6	6	0	3.723139	0.723655	-1.986295
7	6	0	4.011494	-0.923022	0.701176
8	6	0	2.105038	-2.303353	0.050752
9	1	0	1.653982	2.732007	-0.263034
10	1	0	1.409678	2.385552	-1.980794
11	1	0	2.949213	3.111239	-1.432382

12	1	0	3.988738	-0.328331	-1.887331
13	1	0	4.629509	1.331841	-1.887516
14	1	0	3.305214	0.887284	-2.989999
15	1	0	3.883592	-1.194668	1.760018
16	1	0	4.743707	-1.608011	0.255063
17	1	0	2.838202	-3.060042	-0.252410
18	1	0	1.288649	-2.328160	-0.676743
19	1	0	1.733203	-2.558169	1.052436
20	1	0	4.401543	0.094402	0.642234
21	6	0	0.041100	-0.143447	1.091020
22	8	0	0.854887	-0.684750	2.109866
23	8	0	-2.330246	2.517953	1.179390
24	6	0	-3.739908	0.722387	-0.560580
25	6	0	-4.370715	-0.215187	-1.366613
26	6	0	-3.816591	-1.495323	-1.483032
27	6	0	-2.649738	-1.834687	-0.812112
28	6	0	-2.569507	0.392838	0.123543
29	6	0	-2.010095	-0.887483	0.000039
30	6	0	-1.910215	1.387326	0.997076
31	7	0	-0.874784	-1.203195	0.725664
32	7	0	-0.774300	0.932025	1.651882
33	1	0	-0.219809	1.724553	1.968067
34	1	0	-2.226564	-2.831532	-0.910813
35	1	0	-4.299784	-2.238744	-2.111298
36	1	0	-5.281241	0.038608	-1.899142
37	1	0	-4.135478	1.726107	-0.434953
38	1	0	1.152497	0.032201	2.687798
39	1	0	-0.408828	-2.060342	0.462310

TMG-**11**

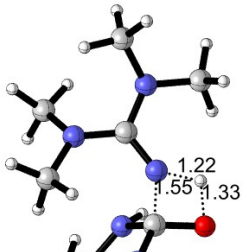
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.400064	1.628480	0.059795
2	6	0	1.933537	0.327347	-0.026001
3	7	0	2.932615	-0.690356	-0.155265



4	7	0	0.681200	0.102505	0.082130
5	6	0	1.435095	2.637535	0.473855
6	6	0	3.324297	2.108998	-0.959270
7	6	0	4.201685	-0.513401	0.540886
8	6	0	3.052997	-1.329260	-1.464418
9	1	0	0.888263	2.287363	1.349729
10	1	0	0.706666	2.851847	-0.320113
11	1	0	1.983775	3.550563	0.722067
12	1	0	3.939528	1.297014	-1.345119
13	1	0	3.982949	2.871950	-0.532772
14	1	0	2.774265	2.551832	-1.803058
15	1	0	4.628411	-1.502937	0.735735
16	1	0	4.938893	0.065529	-0.033580
17	1	0	3.716650	-0.767430	-2.139332
18	1	0	2.066500	-1.410955	-1.924884
19	1	0	3.459679	-2.338187	-1.340600
20	1	0	4.028723	-0.009266	1.492594
21	6	0	0.026931	-1.167725	0.381302
22	8	0	0.859305	-2.270868	0.515573
23	8	0	-2.178935	0.304093	2.773295
24	6	0	-3.638449	0.856378	0.365665
25	6	0	-4.334428	1.018255	-0.825539
26	6	0	-3.889417	0.348170	-1.969558
27	6	0	-2.764371	-0.465856	-1.929559
28	6	0	-2.507537	0.042809	0.419804
29	6	0	-2.056953	-0.623507	-0.731021
30	6	0	-1.801216	-0.163682	1.709784
31	7	0	-0.952124	-1.462616	-0.642478
32	7	0	-0.710124	-0.995835	1.623160
33	1	0	-0.152214	-1.069105	2.467094
34	1	0	-2.427651	-0.984826	-2.823886
35	1	0	-4.425515	0.462830	-2.907825
36	1	0	-5.215046	1.650872	-0.867005
37	1	0	-3.953799	1.346078	1.282697
38	1	0	1.782378	-1.938835	0.515352
39	1	0	-0.519867	-1.711759	-1.525019

TMG-**TS$_{11/12}$**

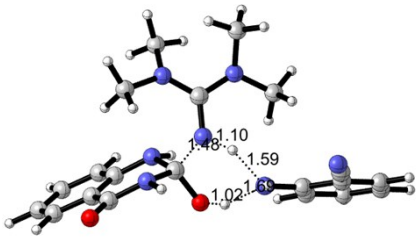


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.645000	0.989433	1.000607
2	6	0	2.196810	0.018238	0.221562
3	7	0	3.471018	0.239393	-0.232412
4	7	0	1.583059	-1.099264	-0.077393
5	6	0	0.536353	0.690459	1.891467
6	6	0	1.827268	2.401074	0.703002
7	6	0	4.476821	0.849541	0.627774
8	6	0	4.006589	-0.618619	-1.277456
9	1	0	0.531003	-0.373005	2.130159
10	1	0	-0.427287	0.963145	1.444747
11	1	0	0.669848	1.268239	2.812736
12	1	0	2.559195	2.528946	-0.094796
13	1	0	2.165562	2.944131	1.593674
14	1	0	0.870158	2.826936	0.374695
15	1	0	5.228539	0.100057	0.907653
16	1	0	4.981426	1.672311	0.109260
17	1	0	4.863716	-0.111609	-1.728577
18	1	0	3.255188	-0.787122	-2.050281
19	1	0	4.335843	-1.588411	-0.880134
20	1	0	4.014122	1.230877	1.537951
21	6	0	0.134670	-1.270115	-0.594173
22	8	0	0.490250	-2.114696	-1.580601
23	8	0	-2.601710	-2.164015	1.621491
24	6	0	-3.775176	0.181542	0.491665
25	6	0	-4.302715	1.298362	-0.140088
26	6	0	-3.532928	1.961628	-1.103286
27	6	0	-2.253818	1.526413	-1.420194
28	6	0	-2.492281	-0.270480	0.177289
29	6	0	-1.716052	0.400072	-0.776849
30	6	0	-1.966493	-1.501372	0.812752
31	7	0	-0.415789	-0.008663	-1.045126
32	7	0	-0.699808	-1.849487	0.433237
33	1	0	-0.400484	-2.774511	0.723502
34	1	0	-1.658783	2.053152	-2.162517
35	1	0	-3.936609	2.832614	-1.612572

36	1	0	-5.300790	1.648843	0.101326
37	1	0	-4.338916	-0.378389	1.232253
38	1	0	1.663744	-1.890141	-1.004365
39	1	0	-0.102435	0.163284	-1.995013

MG-$TS_{11/12}$'



Standard orientation:

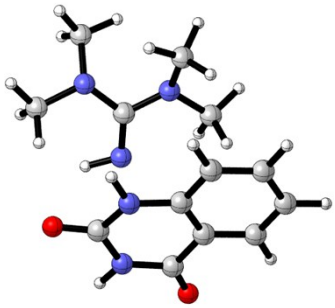
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.104245	2.625193	0.260773
2	6	0	0.027237	1.898741	0.099064
3	7	0	1.134537	2.555333	-0.320714
4	7	0	0.122322	0.597903	0.344458
5	6	0	-2.138537	2.275112	1.223358
6	6	0	-1.497331	3.628222	-0.718772
7	6	0	1.388574	3.942690	0.047057
8	6	0	2.278446	1.845008	-0.886496
9	1	0	-1.712366	1.681065	2.029237
10	1	0	-2.951788	1.710482	0.752766
11	1	0	-2.538062	3.207897	1.634537
12	1	0	-0.763968	3.681815	-1.523956
13	1	0	-1.597590	4.616425	-0.254965
14	1	0	-2.465966	3.339332	-1.144254
15	1	0	2.368964	4.003363	0.530896
16	1	0	1.393950	4.591296	-0.836348
17	1	0	2.762967	2.505013	-1.611226
18	1	0	1.949025	0.938672	-1.396219
19	1	0	3.003468	1.564652	-0.112548
20	1	0	0.629700	4.291748	0.747453
21	6	0	-0.904436	-0.454193	0.162320
22	8	0	-0.242328	-1.569611	-0.305987
23	8	0	-3.181168	-1.699197	2.657318
24	6	0	-4.973008	-1.650883	0.426373
25	6	0	-5.781466	-1.590126	-0.699282
26	6	0	-5.273125	-1.025472	-1.874354
27	6	0	-3.980150	-0.521823	-1.923197

28	6	0	-3.669238	-1.152372	0.387534
29	6	0	-3.163498	-0.583628	-0.786597
30	6	0	-2.810311	-1.239224	1.590986
31	7	0	-1.879639	-0.023010	-0.809470
32	7	0	-1.555194	-0.693049	1.438098
33	1	0	-0.914044	-0.919131	2.194067
34	1	0	-3.593527	-0.082211	-2.839542
35	1	0	-5.892979	-0.979886	-2.765321
36	1	0	-6.793602	-1.979790	-0.671734
37	1	0	-5.320112	-2.086348	1.358811
38	1	0	-1.452336	-0.061040	-1.731119
39	1	0	1.101715	0.119783	0.509569
40	7	0	2.126913	-1.059252	0.784636
41	1	0	0.665838	-1.632970	0.163991
42	6	0	3.211717	-1.210074	-0.020247
43	6	0	4.561352	-1.047924	0.413913
44	6	0	3.043550	-1.510730	-1.400488
45	6	0	4.123161	-1.646391	-2.253374
46	6	0	5.443195	-1.494888	-1.797241
47	6	0	5.648488	-1.197698	-0.460889
48	6	0	4.784693	-0.687154	1.781627
49	7	0	4.909882	-0.371669	2.891980
50	1	0	2.030923	-1.664973	-1.767688
51	1	0	3.941791	-1.890527	-3.297530
52	1	0	6.282572	-1.615027	-2.473520
53	1	0	6.653344	-1.070766	-0.067473
54	1	0	2.402126	-1.001701	1.765370

TMG-**12**

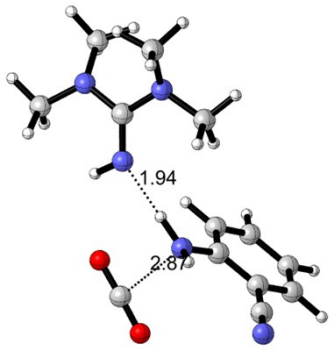
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.601311	-1.512619	0.724603



2	6	0	-1.872661	-0.160412	0.621307
3	7	0	-3.031985	0.138712	-0.115954
4	7	0	-1.079420	0.694025	1.168638
5	6	0	-0.528937	-1.922142	1.612380
6	6	0	-1.864301	-2.435130	-0.365249
7	6	0	-4.261671	-0.553581	0.259730
8	6	0	-3.267230	1.540681	-0.418224
9	1	0	-0.526433	-1.286995	2.497833
10	1	0	0.454667	-1.842775	1.128420
11	1	0	-0.698555	-2.964683	1.902013
12	1	0	-2.445609	-1.944237	-1.146975
13	1	0	-2.417573	-3.313080	-0.006735
14	1	0	-0.916979	-2.785467	-0.799008
15	1	0	-4.768494	-0.033631	1.087732
16	1	0	-4.940712	-0.581135	-0.598707
17	1	0	-4.050653	1.601753	-1.179183
18	1	0	-2.363006	2.012177	-0.810783
19	1	0	-3.608694	2.106996	0.465006
20	1	0	-4.050709	-1.574495	0.576297
21	6	0	0.528563	2.179129	-0.743274
22	8	0	-0.266432	3.054098	-1.038728
23	8	0	2.951905	1.562100	1.796112
24	6	0	3.035526	-1.010047	0.502121
25	6	0	2.991288	-2.221278	-0.173568
26	6	0	2.128215	-2.366378	-1.266545
27	6	0	1.326105	-1.314916	-1.688761
28	6	0	2.229796	0.053578	0.091533
29	6	0	1.377276	-0.092340	-1.009184
30	6	0	2.266248	1.338064	0.819692
31	7	0	0.610398	0.986717	-1.422549
32	7	0	1.455625	2.326495	0.271163
33	1	0	1.397982	3.198457	0.786859
34	1	0	0.662432	-1.430596	-2.542164
35	1	0	2.083260	-3.312734	-1.798406
36	1	0	3.616064	-3.050178	0.142115
37	1	0	3.683328	-0.854743	1.360036
38	1	0	-1.492991	1.625723	1.171799
39	1	0	-0.103555	0.855364	-2.128275

TMG-**13**

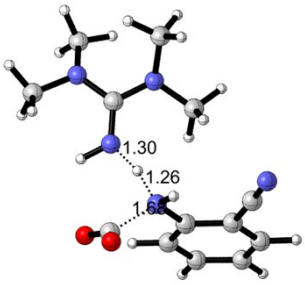


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.907102	-0.278709	-0.003254
2	6	0	1.374081	0.013356	1.269253
3	6	0	2.119320	-0.213869	2.415819
4	6	0	3.416645	-0.737006	2.350538
5	6	0	3.215435	-0.811543	-0.058695
6	6	0	3.956426	-1.034347	1.109177
7	1	0	3.990486	-0.909169	3.254618
8	1	0	1.681847	0.020437	3.382750
9	7	0	1.196534	0.013181	-1.138349
10	1	0	1.527145	-0.380383	-2.010846
11	1	0	4.958270	-1.443387	1.019766
12	1	0	0.178875	0.113132	-1.038860
13	1	0	-1.697813	1.513706	-0.291504
14	7	0	-3.959713	0.491919	0.053484
15	6	0	-2.724554	-0.111946	-0.184487
16	7	0	-2.741093	-1.497516	-0.136469
17	7	0	-1.624783	0.509994	-0.443460
18	6	0	-4.056433	1.918927	-0.181980
19	6	0	-4.751440	0.042087	1.193734
20	6	0	-3.816605	-2.215775	-0.810585
21	6	0	-1.454296	-2.163845	-0.246478
22	1	0	-3.624737	2.169231	-1.153879
23	1	0	-3.555103	2.512843	0.599939
24	1	0	-5.113830	2.196620	-0.193249
25	1	0	-4.534311	-1.001938	1.416871
26	1	0	-5.817917	0.147541	0.968132
27	1	0	-4.522756	0.641585	2.087875
28	1	0	-3.537875	-2.445847	-1.849966
29	1	0	-4.012456	-3.157746	-0.288098
30	1	0	-1.589123	-3.214860	0.023833
31	1	0	-0.735779	-1.708562	0.437140
32	1	0	-1.048653	-2.107527	-1.267777
33	1	0	-4.728043	-1.619249	-0.824884

34	6	0	1.588771	2.778469	-0.464407
35	8	0	0.451778	2.860398	-0.220047
36	8	0	2.725949	2.738394	-0.694518
37	1	0	0.367654	0.420519	1.326710
38	6	0	3.764452	-1.121879	-1.346002
39	7	0	4.151752	-1.363406	-2.412042

TMG-**TS$_{13/14}$**

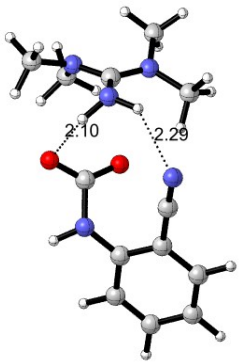


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.940275	0.274301	0.140514
2	6	0	2.007545	0.793504	1.439534
3	6	0	2.887852	0.244183	2.365012
4	6	0	3.710548	-0.835213	2.032555
5	6	0	2.757494	-0.827427	-0.184717
6	6	0	3.640328	-1.373529	0.756266
7	1	0	4.396752	-1.251799	2.762438
8	1	0	2.935545	0.669981	3.363195
9	7	0	1.024440	0.802341	-0.798388
10	1	0	1.197539	0.447474	-1.740246
11	1	0	4.257969	-2.218917	0.469635
12	1	0	-0.146892	0.595506	-0.380775
13	1	0	-1.506067	1.592181	0.529008
14	7	0	-3.629069	0.203324	0.323722
15	6	0	-2.323317	-0.178826	0.140256
16	7	0	-2.091813	-1.505689	-0.089203
17	7	0	-1.326036	0.659008	0.169763
18	6	0	-3.950515	1.620896	0.299554
19	6	0	-4.540180	-0.609613	1.121669
20	6	0	-2.997988	-2.302750	-0.907521
21	6	0	-0.721291	-1.994486	-0.047614
22	1	0	-3.413930	2.115640	-0.512330
23	1	0	-3.709736	2.117895	1.250892
24	1	0	-5.023353	1.725906	0.119318
25	1	0	-4.108500	-1.592661	1.307092

26	1	0	-5.498849	-0.729009	0.605421
27	1	0	-4.721839	-0.124085	2.089437
28	1	0	-2.498900	-2.577613	-1.844903
29	1	0	-3.284873	-3.221423	-0.383712
30	1	0	-0.746423	-3.072665	0.131730
31	1	0	-0.178804	-1.510986	0.767228
32	1	0	-0.192221	-1.812649	-0.994119
33	1	0	-3.893953	-1.731169	-1.149556
34	6	0	0.912935	2.473668	-0.952093
35	8	0	0.470804	2.950116	0.081958
36	8	0	1.239919	2.797661	-2.069505
37	1	0	1.380247	1.641770	1.689729
38	6	0	2.641122	-1.424794	-1.486428
39	7	0	2.491284	-1.902566	-2.531754

TMG-**14**

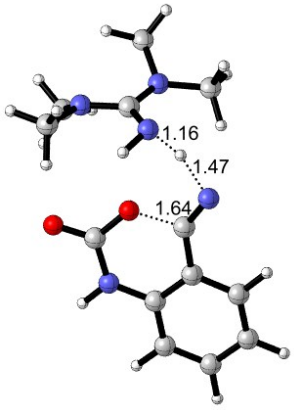


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.398456	-0.642229	-0.027416
2	6	0	4.430230	-1.275858	-0.723756
3	6	0	5.650577	-0.638285	-0.920901
4	6	0	5.855361	0.656088	-0.443823
5	6	0	3.620432	0.647646	0.486535
6	6	0	4.841113	1.293998	0.259238
7	1	0	6.801830	1.160114	-0.609630
8	1	0	6.438908	-1.149550	-1.465289
9	7	0	2.179952	-1.302666	0.184730
10	1	0	2.194429	-2.306741	0.306417
11	1	0	4.985768	2.291703	0.661414
12	1	0	-1.598111	0.725402	-0.764383
13	1	0	-0.911353	-1.150292	-0.181732
14	7	0	-4.048682	-0.939015	0.449699
15	6	0	-3.341507	0.044961	-0.215901
16	7	0	-4.083945	1.158291	-0.592135
17	7	0	-2.084454	-0.114237	-0.456569

18	6	0	-3.273430	-2.040826	0.994721
19	6	0	-5.361454	-1.335257	-0.044172
20	6	0	-4.980358	1.770117	0.383929
21	6	0	-3.435477	2.125172	-1.459049
22	1	0	-2.420194	-1.655406	1.554704
23	1	0	-2.901124	-2.711785	0.206347
24	1	0	-3.917589	-2.610079	1.670439
25	1	0	-5.834489	-0.511354	-0.577623
26	1	0	-5.998078	-1.630786	0.796274
27	1	0	-5.274522	-2.188835	-0.732882
28	1	0	-4.467178	2.575614	0.929152
29	1	0	-5.849584	2.195122	-0.129026
30	1	0	-4.200056	2.795586	-1.860365
31	1	0	-2.950875	1.614418	-2.293952
32	1	0	-2.688136	2.733993	-0.926018
33	1	0	-5.319120	1.028498	1.106529
34	6	0	0.952528	-0.760571	-0.174759
35	8	0	0.826525	0.366560	-0.613251
36	8	0	-0.022088	-1.633316	0.023473
37	1	0	4.258119	-2.270288	-1.126569
38	6	0	2.646132	1.290943	1.327446
39	7	0	1.922880	1.823816	2.057399

TMG-**TS$_{14/15}$**



Standard orientation:

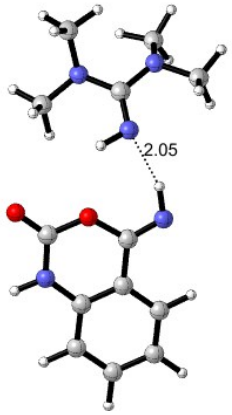
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.636201	-0.027698	2.025473
2	1	0	0.990477	-1.423025	1.301631
3	7	0	3.054937	0.861422	0.240079
4	6	0	2.606585	-0.413868	0.386697
5	7	0	2.868065	-1.301283	-0.604689
6	7	0	1.962978	-0.819292	1.478089
7	6	0	2.939854	1.781586	1.364912
8	6	0	2.970015	1.527703	-1.065263
9	6	0	4.094308	-1.208983	-1.390845

10	6	0	2.310979	-2.648483	-0.523528
11	1	0	3.288673	1.302335	2.282667
12	1	0	1.909258	2.144970	1.474298
13	1	0	3.588101	2.637377	1.162133
14	1	0	2.626881	0.826970	-1.826028
15	1	0	3.944899	1.936175	-1.354647
16	1	0	2.230165	2.330889	-0.990068
17	1	0	4.696230	-2.107348	-1.209373
18	1	0	3.871660	-1.148206	-2.461639
19	1	0	2.426322	-3.114659	-1.504445
20	1	0	1.250306	-2.619366	-0.277247
21	1	0	2.843583	-3.247619	0.227323
22	1	0	4.679164	-0.339329	-1.093991
23	6	0	-2.872822	0.695762	-0.225326
24	6	0	-4.220129	0.876105	-0.562127
25	6	0	-5.105940	-0.190090	-0.494500
26	6	0	-4.664168	-1.452656	-0.089968
27	6	0	-2.421652	-0.567204	0.180366
28	6	0	-3.329086	-1.629341	0.246795
29	1	0	-5.356992	-2.286113	-0.035434
30	1	0	-6.147852	-0.033841	-0.758848
31	7	0	-1.997475	1.774595	-0.285077
32	1	0	-2.349316	2.689688	-0.531578
33	1	0	-2.949168	-2.591832	0.575981
34	6	0	-0.635883	1.709967	-0.060082
35	8	0	0.058441	2.714609	-0.149444
36	8	0	-0.158121	0.526436	0.241366
37	1	0	-4.564208	1.858596	-0.875844
38	6	0	-1.026671	-0.820971	0.573256
39	7	0	-0.415546	-1.754512	1.041876

TMG-**15**

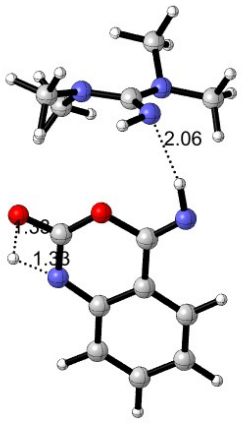
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.276978	-1.531269	-0.491969



2	6	0	3.503359	0.579232	0.093622
3	6	0	4.885549	0.641304	0.283035
4	6	0	5.615599	-0.538581	0.348734
5	6	0	4.980652	-1.778626	0.227432
6	6	0	2.860006	-0.653224	-0.028299
7	6	0	3.606031	-1.831721	0.039067
8	1	0	5.559235	-2.695049	0.278631
9	1	0	6.690466	-0.490414	0.495780
10	7	0	2.733705	1.740928	0.023700
11	1	0	3.170088	2.648996	0.116011
12	1	0	3.077539	-2.774616	-0.060889
13	6	0	1.377780	1.769986	-0.159709
14	8	0	0.729601	2.786098	-0.209282
15	8	0	0.768250	0.566300	-0.286626
16	1	0	5.377366	1.605742	0.378050
17	6	0	1.401443	-0.689206	-0.229660
18	7	0	0.724434	-1.738173	-0.350766
19	1	0	-1.497382	0.406361	-1.025334
20	7	0	-3.540112	1.028745	0.252134
21	6	0	-3.112355	-0.217468	-0.214970
22	7	0	-4.012847	-1.254706	0.005031
23	7	0	-1.990763	-0.455379	-0.799031
24	6	0	-4.885421	1.469716	-0.096320
25	6	0	-2.564593	2.103785	0.230375
26	6	0	-4.633814	-1.375457	1.317393
27	6	0	-3.657387	-2.537784	-0.575110
28	1	0	-5.558441	0.615890	-0.171598
29	1	0	-4.888509	1.999058	-1.062157
30	1	0	-5.258217	2.153728	0.673445
31	1	0	-1.617374	1.771867	0.659590
32	1	0	-2.947696	2.931170	0.834133
33	1	0	-2.370261	2.483178	-0.786174
34	1	0	-5.609434	-1.862761	1.217151
35	1	0	-4.009724	-1.982497	1.991637
36	1	0	-2.838351	-3.024839	-0.024550
37	1	0	-3.336567	-2.397805	-1.607345
38	1	0	-4.539866	-3.184073	-0.547437
39	1	0	-4.770717	-0.393481	1.769281

TMG-**TS$_{15/16}$**

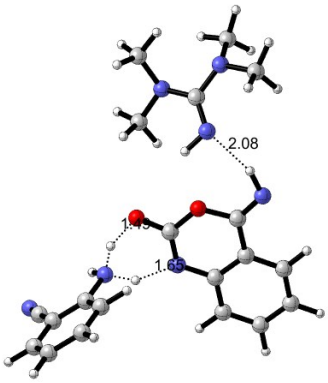


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.161129	0.067956	-2.105636
2	1	0	-0.489659	-1.483722	-1.520479
3	7	0	-2.971197	0.965835	0.048565
4	6	0	-2.755340	-0.347791	-0.345312
5	7	0	-2.952806	-1.292958	0.660350
6	7	0	-2.411418	-0.733592	-1.528375
7	6	0	-2.977042	1.991989	-0.976097
8	6	0	-2.507911	1.431033	1.352184
9	6	0	-4.178392	-1.195594	1.446861
10	6	0	-2.635807	-2.668873	0.308306
11	1	0	-3.600606	1.677083	-1.817077
12	1	0	-1.965484	2.235782	-1.333793
13	1	0	-3.411604	2.900506	-0.549775
14	1	0	-2.210201	0.580581	1.966160
15	1	0	-3.303077	1.984470	1.867614
16	1	0	-1.645632	2.098167	1.227515
17	1	0	-5.015492	-1.691307	0.930934
18	1	0	-4.027953	-1.685539	2.413947
19	1	0	-2.697659	-3.272205	1.218450
20	1	0	-1.623517	-2.735750	-0.089978
21	1	0	-3.332219	-3.068675	-0.442376
22	1	0	-4.450901	-0.155107	1.619019
23	6	0	2.935526	0.639136	0.257597
24	6	0	4.242760	0.694295	0.743616
25	6	0	5.023526	-0.454334	0.727289
26	6	0	4.514222	-1.659426	0.230329
27	6	0	2.414271	-0.566324	-0.242690
28	6	0	3.213959	-1.712421	-0.253599
29	1	0	5.132769	-2.550841	0.221998
30	1	0	6.040906	-0.412145	1.105171
31	7	0	2.103761	1.753110	0.247335
32	1	0	1.550859	2.960992	0.347143
33	1	0	2.790009	-2.631123	-0.646906

34	6	0	0.874776	1.664605	-0.213326
35	8	0	0.316453	2.807385	-0.126511
36	8	0	0.286433	0.589242	-0.689014
37	1	0	4.625290	1.635398	1.125470
38	6	0	1.032642	-0.633787	-0.758136
39	7	0	0.487242	-1.652764	-1.238635

TMG-**TS$_{15/16}$'**



Standard orientation:

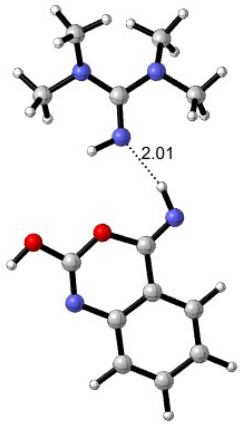
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.624361	-0.758302	0.934918
2	7	0	-3.957322	-2.288067	-0.514434
3	6	0	-4.364591	-1.212245	0.282891
4	7	0	-5.743806	-1.015806	0.319342
5	7	0	-3.588063	-0.427968	0.941309
6	6	0	-4.624208	-3.570246	-0.324535
7	6	0	-2.530710	-2.416375	-0.747125
8	6	0	-6.472990	-1.033639	-0.942638
9	6	0	-6.204602	0.027981	1.219241
10	1	0	-5.667105	-3.418077	-0.046717
11	1	0	-4.135679	-4.155065	0.471034
12	1	0	-4.581022	-4.147856	-1.254141
13	1	0	-2.103735	-1.457870	-1.048304
14	1	0	-2.376042	-3.137772	-1.554667
15	1	0	-1.983069	-2.771702	0.141256
16	1	0	-7.522467	-1.278836	-0.750131
17	1	0	-6.429978	-0.050028	-1.436699
18	1	0	-5.964847	1.032631	0.839376
19	1	0	-5.728347	-0.089113	2.192475
20	1	0	-7.289625	-0.065373	1.325486
21	1	0	-6.052600	-1.775544	-1.620971
22	7	0	2.870441	-0.908371	-0.959443
23	1	0	-3.013222	1.566325	0.777740
24	6	0	1.076254	2.491295	-0.425567
25	6	0	2.118241	3.385662	-0.712095

26	6	0	1.908198	4.753950	-0.624479
27	6	0	0.657872	5.261792	-0.249373
28	6	0	-0.173107	3.004559	-0.050288
29	6	0	-0.377920	4.384256	0.036904
30	1	0	0.500222	6.333613	-0.183063
31	1	0	2.723572	5.435688	-0.850502
32	7	0	1.303609	1.122138	-0.518129
33	1	0	-1.361143	4.737029	0.333131
34	6	0	0.316054	0.285560	-0.248257
35	8	0	0.428920	-0.971184	-0.306294
36	8	0	-0.918062	0.709944	0.127534
37	1	0	3.085262	2.985242	-1.004443
38	6	0	-1.260067	2.064445	0.254531
39	7	0	-2.421473	2.392186	0.609774
40	1	0	2.561305	0.144414	-0.941201
41	1	0	1.825505	-1.239883	-0.740444
42	1	0	3.198869	-1.206937	-1.880024
43	6	0	3.776603	-1.220179	0.112057
44	6	0	3.423290	-0.861022	1.408747
45	6	0	4.287482	-1.158206	2.458653
46	6	0	5.498007	-1.811934	2.223286
47	6	0	5.852188	-2.170580	0.929289
48	6	0	4.990301	-1.873440	-0.132947
49	1	0	4.010107	-0.877720	3.469823
50	1	0	6.164114	-2.041588	3.048226
51	1	0	6.788712	-2.678634	0.724348
52	6	0	5.329149	-2.227423	-1.484287
53	1	0	2.477535	-0.355353	1.581370
54	7	0	5.544975	-2.483346	-2.592969

TMG-**16**

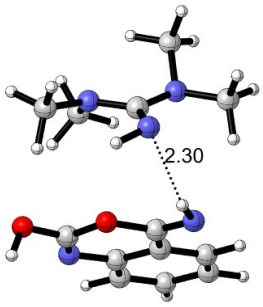
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	1	0	-0.276873	-1.225180	0.029775
2	6	0	3.693754	0.580221	-0.004401
3	6	0	5.091660	0.525563	-0.011304
4	6	0	5.736069	-0.703776	-0.005802
5	6	0	4.999474	-1.894794	0.006573
6	6	0	2.958336	-0.613492	0.008241
7	6	0	3.612532	-1.847961	0.013565
8	1	0	5.511345	-2.852095	0.010834
9	1	0	6.821757	-0.739922	-0.011223
10	7	0	3.060552	1.830440	-0.010482
11	1	0	1.693877	3.673683	-0.019454
12	1	0	3.009179	-2.750435	0.023122
13	6	0	1.786627	1.814351	-0.003152
14	8	0	1.061535	2.935714	-0.008177
15	8	0	0.965657	0.762485	0.010090
16	1	0	5.645889	1.458865	-0.021040
17	6	0	1.489934	-0.551902	0.016110
18	7	0	0.708398	-1.532659	0.027453
19	1	0	-1.597433	0.846416	-0.109485
20	7	0	-4.099988	0.925050	0.134892
21	6	0	-3.234834	-0.163464	-0.023210
22	7	0	-3.873976	-1.391960	-0.146637
23	7	0	-1.950756	-0.106429	-0.049228
24	6	0	-5.227240	1.048697	-0.782620
25	6	0	-3.493414	2.200065	0.462087
26	6	0	-4.948480	-1.711752	0.785475
27	6	0	-3.010034	-2.527207	-0.426495
28	1	0	-5.561480	0.063246	-1.105481
29	1	0	-4.944908	1.627627	-1.675568
30	1	0	-6.054692	1.563439	-0.282920
31	1	0	-2.782156	2.078611	1.282316
32	1	0	-4.281349	2.885547	0.786397
33	1	0	-2.973947	2.656490	-0.397028
34	1	0	-5.626861	-2.436581	0.324176
35	1	0	-4.547077	-2.151037	1.711915
36	1	0	-2.395409	-2.800244	0.443988
37	1	0	-2.342259	-2.288735	-1.254929
38	1	0	-3.640496	-3.377747	-0.700873
39	1	0	-5.510569	-0.815932	1.047788

TMG-**TS$_{16/17}$**

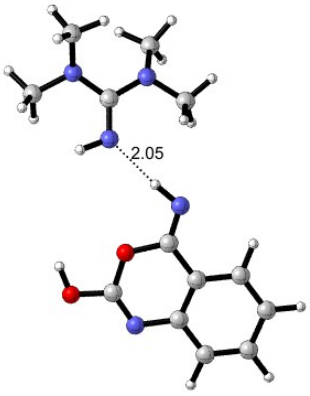


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.734872	0.752429	-1.745094
2	1	0	-0.697976	-0.704751	-2.331798
3	7	0	-2.478150	0.785554	0.709620
4	6	0	-2.532196	-0.292995	-0.170600
5	7	0	-2.328938	-1.532826	0.430340
6	7	0	-2.760668	-0.218869	-1.437505
7	6	0	-2.933219	2.074560	0.229854
8	6	0	-1.441084	0.849462	1.731278
9	6	0	-3.042166	-1.812288	1.672194
10	6	0	-2.323155	-2.679281	-0.466849
11	1	0	-3.892983	1.962575	-0.281814
12	1	0	-2.207354	2.553014	-0.444320
13	1	0	-3.079247	2.731999	1.091897
14	1	0	-0.857849	-0.073828	1.730768
15	1	0	-1.875690	0.995615	2.728823
16	1	0	-0.766858	1.693588	1.536170
17	1	0	-4.070575	-2.149919	1.467500
18	1	0	-2.519332	-2.605419	2.215170
19	1	0	-2.022369	-3.557494	0.111506
20	1	0	-1.606343	-2.522763	-1.271398
21	1	0	-3.316083	-2.854116	-0.905453
22	1	0	-3.092686	-0.928302	2.305799
23	6	0	2.573742	0.563057	0.258707
24	6	0	3.752225	0.342712	0.978503
25	6	0	4.334775	-0.917188	0.976297
26	6	0	3.752438	-1.968745	0.257539
27	6	0	1.994145	-0.489201	-0.461066
28	6	0	2.584170	-1.755444	-0.460998
29	1	0	4.214320	-2.951203	0.262015
30	1	0	5.250013	-1.087525	1.535835
31	7	0	2.005061	1.846904	0.270197
32	1	0	0.492901	3.702168	-1.129395

33	1	0	2.109079	-2.549060	-1.029200
34	6	0	0.916291	1.991882	-0.359832
35	8	0	0.242485	3.162727	-0.363054
36	8	0	0.228071	1.053105	-1.047224
37	1	0	4.187079	1.173047	1.526002
38	6	0	0.759393	-0.236139	-1.215323
39	7	0	0.184153	-1.070631	-1.959655

TMG-**17**

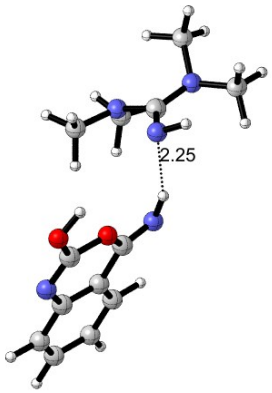


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.379413	-0.432534	-0.255753
2	6	0	3.905234	0.432436	0.066028
3	6	0	5.253140	0.056076	0.100641
4	6	0	5.603247	-1.280858	-0.021011
5	6	0	4.618128	-2.264422	-0.179455
6	6	0	2.921493	-0.554694	-0.093192
7	6	0	3.280005	-1.900150	-0.215803
8	1	0	4.900213	-3.308453	-0.273915
9	1	0	6.651251	-1.565602	0.006985
10	7	0	3.583830	1.788273	0.195631
11	1	0	0.963200	3.350355	0.235025
12	1	0	2.491278	-2.635933	-0.338131
13	6	0	2.349866	2.075215	0.157252
14	8	0	1.932609	3.337323	0.274137
15	8	0	1.301722	1.234670	0.003410
16	1	0	6.000626	0.833001	0.225260
17	6	0	1.508366	-0.156275	-0.127497
18	7	0	0.526772	-0.926619	-0.259291
19	1	0	-2.282557	1.368346	-0.609664
20	7	0	-4.605297	0.703228	0.005565
21	6	0	-3.438156	-0.064552	-0.088205
22	7	0	-3.633386	-1.421815	0.095343
23	7	0	-2.254582	0.394337	-0.316033
24	6	0	-5.778356	0.275842	-0.749279

25	6	0	-4.450050	2.142228	0.047047
26	6	0	-4.498920	-1.884682	1.171843
27	6	0	-2.486052	-2.284579	-0.134033
28	1	0	-5.780112	-0.807828	-0.862511
29	1	0	-5.785858	0.728665	-1.752841
30	1	0	-6.688299	0.582958	-0.222764
31	1	0	-3.679686	2.414625	0.772623
32	1	0	-5.396798	2.584640	0.369352
33	1	0	-4.191407	2.572229	-0.935615
34	1	0	-4.996192	-2.813307	0.871712
35	1	0	-3.912859	-2.084050	2.081546
36	1	0	-1.747330	-2.214636	0.676858
37	1	0	-1.991521	-2.008991	-1.065901
38	1	0	-2.844333	-3.315805	-0.203914
39	1	0	-5.253895	-1.134970	1.406749

TMG-**TS$_{17/18}$**



Standard orientation:

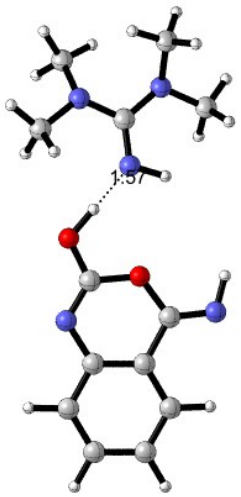
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.990885	1.529783	-1.396486
2	1	0	-0.773245	-0.231203	-1.164744
3	7	0	-4.120171	-0.474838	-0.437928
4	6	0	-3.005750	0.236478	0.010431
5	7	0	-2.510092	-0.195627	1.229127
6	7	0	-2.422424	1.202638	-0.617438
7	6	0	-4.561779	-0.243034	-1.796900
8	6	0	-5.208658	-0.753814	0.490003
9	6	0	-2.335730	-1.622584	1.475748
10	6	0	-1.504060	0.629290	1.871454
11	1	0	-3.708969	-0.274319	-2.479691
12	1	0	-5.085344	0.720400	-1.915901
13	1	0	-5.254757	-1.040972	-2.077831
14	1	0	-4.834162	-0.772244	1.512971
15	1	0	-5.658870	-1.724727	0.255754
16	1	0	-5.989686	0.018541	0.419151

17	1	0	-1.306360	-1.927927	1.238760
18	1	0	-2.539044	-1.843398	2.529664
19	1	0	-1.481081	0.377231	2.936349
20	1	0	-1.760511	1.681701	1.747961
21	1	0	-0.504289	0.460803	1.448379
22	1	0	-3.015769	-2.201669	0.851074
23	6	0	3.336470	0.312406	0.083801
24	6	0	4.629261	-0.134701	0.382658
25	6	0	4.960999	-1.469836	0.203779
26	6	0	4.012354	-2.385187	-0.271934
27	6	0	2.389336	-0.608420	-0.393249
28	6	0	2.727640	-1.953835	-0.567179
29	1	0	4.281234	-3.427838	-0.409454
30	1	0	5.967014	-1.807332	0.436524
31	7	0	3.030211	1.662911	0.284953
32	1	0	0.511388	3.325142	-0.188130
33	1	0	1.967920	-2.635481	-0.937627
34	6	0	1.860967	2.022168	-0.053204
35	8	0	1.444470	3.278534	0.083790
36	8	0	0.883177	1.255121	-0.582609
37	1	0	5.349168	0.587628	0.754001
38	6	0	1.037024	-0.129843	-0.694279
39	7	0	0.047708	-0.834780	-1.032563

TMG-**18**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.729991	1.193764	-0.112148
2	1	0	-1.018727	2.805376	-0.261069
3	7	0	4.209591	1.100608	0.210199
4	6	0	3.308411	0.070571	-0.019170
5	7	0	3.863414	-1.172711	-0.198063
6	7	0	2.021555	0.222021	-0.064440
7	6	0	3.683557	2.379782	0.645656
8	6	0	5.402942	1.210342	-0.622370

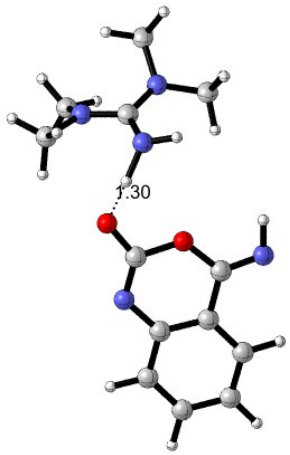


9	6	0	4.991885	-1.608272	0.614482
10	6	0	2.986883	-2.253896	-0.622562
11	1	0	2.946520	2.233159	1.438265
12	1	0	3.224404	2.949576	-0.178440
13	1	0	4.508419	2.973656	1.048371
14	1	0	5.627919	0.251836	-1.089099
15	1	0	6.258688	1.523487	-0.014685
16	1	0	5.247949	1.953941	-1.417124
17	1	0	4.647538	-2.299588	1.395750
18	1	0	5.727080	-2.129126	-0.008964
19	1	0	3.610045	-3.063389	-1.012673
20	1	0	2.318521	-1.903910	-1.410135
21	1	0	2.376340	-2.638360	0.205492
22	1	0	5.470088	-0.755701	1.095783
23	6	0	-3.409050	-0.804779	0.081453
24	6	0	-4.633701	-1.486844	0.149636
25	6	0	-5.826706	-0.784251	0.089329
26	6	0	-5.831621	0.612711	-0.040742
27	6	0	-3.422395	0.593091	-0.047513
28	6	0	-4.629335	1.298378	-0.108601
29	1	0	-6.771670	1.153521	-0.087800
30	1	0	-6.768690	-1.323205	0.143364
31	7	0	-2.229051	-1.539040	0.142091
32	1	0	0.820676	-0.781801	0.053072
33	1	0	-4.592925	2.378871	-0.209011
34	6	0	-1.132245	-0.886435	0.080444
35	8	0	0.036347	-1.459577	0.123424
36	8	0	-1.018959	0.477814	-0.037656
37	1	0	-4.611706	-2.567438	0.249741
38	6	0	-2.139502	1.292741	-0.115967
39	7	0	-2.006124	2.546351	-0.235399

TMG-**TS$_{18/19}$**

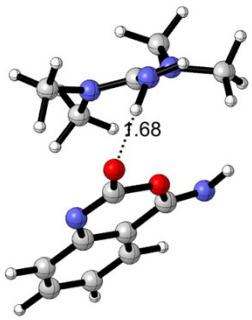
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	1	0	1.943857	1.153480	-1.423407
2	1	0	-0.951556	2.831191	-0.901948
3	7	0	3.700172	1.134971	0.391099
4	6	0	3.076761	0.071376	-0.200103
5	7	0	3.488043	-1.175180	0.138271
6	7	0	2.104830	0.218769	-1.069633
7	6	0	3.073684	2.445720	0.347684
8	6	0	5.139157	1.140976	0.622086
9	6	0	3.920632	-1.499932	1.491365
10	6	0	3.083014	-2.324878	-0.668184
11	1	0	1.993804	2.348455	0.479637
12	1	0	3.285798	2.977013	-0.591777
13	1	0	3.467327	3.043512	1.173837
14	1	0	5.565777	0.172957	0.359462
15	1	0	5.365413	1.361975	1.671051
16	1	0	5.608584	1.908256	-0.006104
17	1	0	3.225102	-2.228891	1.922109
18	1	0	4.925791	-1.936901	1.484450
19	1	0	3.856542	-3.091569	-0.568642
20	1	0	3.001187	-2.026488	-1.714013
21	1	0	2.115409	-2.722074	-0.344304
22	1	0	3.918042	-0.608516	2.118484
23	6	0	-3.073198	-0.824668	0.067817
24	6	0	-4.218645	-1.526013	0.488817
25	6	0	-5.376996	-0.844345	0.820945
26	6	0	-5.435060	0.556629	0.745208
27	6	0	-3.142770	0.577506	-0.004089
28	6	0	-4.316981	1.262053	0.331800
29	1	0	-6.348395	1.082206	1.006099
30	1	0	-6.252586	-1.402662	1.142037
31	7	0	-1.934877	-1.543437	-0.252929
32	1	0	1.191046	-0.542333	-1.094739
33	1	0	-4.321657	2.345383	0.257068
34	6	0	-0.893765	-0.887582	-0.642301
35	8	0	0.224460	-1.398059	-0.969533
36	8	0	-0.863863	0.508897	-0.751126
37	1	0	-4.159760	-2.608826	0.540950
38	6	0	-1.950974	1.298683	-0.446745
39	7	0	-1.875831	2.562586	-0.559776

TMG-**19**



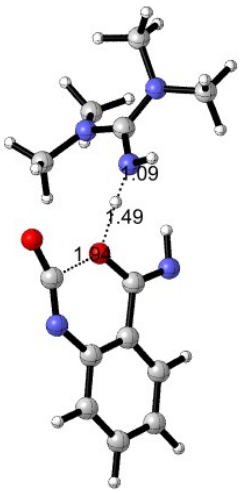
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.573922	0.609264	-1.281365
2	1	0	-0.588606	-2.204981	-1.777492
3	6	0	2.214013	0.698443	-0.208457
4	6	0	3.421084	1.038369	0.439060
5	6	0	4.308245	0.054633	0.838900
6	6	0	4.031109	-1.304721	0.613314
7	6	0	1.947000	-0.666912	-0.423359
8	6	0	2.850280	-1.658047	-0.017692
9	1	0	4.736827	-2.067655	0.926927
10	1	0	5.234308	0.339368	1.332048
11	7	0	1.345832	1.707921	-0.561207
12	1	0	2.599072	-2.696152	-0.215011
13	6	0	0.246930	1.404144	-1.203170
14	8	0	-0.641124	2.183032	-1.586370
15	8	0	-0.082518	0.038840	-1.485056
16	1	0	3.626798	2.091682	0.604591
17	6	0	0.686758	-1.015548	-1.074720
18	7	0	0.288190	-2.215823	-1.254659
19	1	0	-2.173467	1.649628	-1.163934
20	7	0	-1.560964	0.846684	1.198710
21	6	0	-2.357589	0.271981	0.287967
22	7	0	-2.651322	-1.041992	0.364376
23	7	0	-2.877484	1.034640	-0.686036
24	6	0	-1.526863	2.300688	1.379868
25	6	0	-0.477725	0.120893	1.862128
26	6	0	-2.733961	-1.767851	1.625033
27	6	0	-3.088716	-1.779773	-0.811808
28	1	0	-2.461329	2.734345	1.025063
29	1	0	-0.686001	2.736039	0.829434
30	1	0	-1.414656	2.498090	2.449989
31	1	0	-0.300138	-0.835842	1.367606
32	1	0	-0.699063	-0.041175	2.923091

33	1	0	0.430283	0.724367	1.774955
34	1	0	-3.688651	-2.303780	1.654454
35	1	0	-1.917257	-2.491583	1.719212
36	1	0	-2.703404	-2.800504	-0.737237
37	1	0	-2.675562	-1.322453	-1.713045
38	1	0	-4.184033	-1.821892	-0.879580
39	1	0	-2.705217	-1.069548	2.461038

TMG-**TS$_{19/20}$**

Standard orientation:



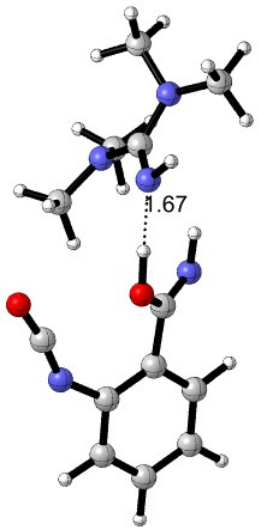
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.886736	-0.057799	-2.012655
2	1	0	-0.335738	-1.835296	0.602047
3	6	0	3.271891	0.568571	-0.242129
4	6	0	4.671269	0.642107	-0.329461
5	6	0	5.463762	-0.458181	-0.040245
6	6	0	4.872907	-1.666035	0.342186
7	6	0	2.674752	-0.646525	0.143980
8	6	0	3.490477	-1.748009	0.429357
9	1	0	5.486833	-2.531882	0.571838
10	1	0	6.544941	-0.375634	-0.113005
11	7	0	2.584215	1.738211	-0.569105
12	1	0	2.997942	-2.669296	0.724130
13	6	0	1.360221	1.952847	-0.544670
14	8	0	0.420520	2.656909	-0.716515
15	8	0	0.515757	0.333062	0.094125
16	1	0	5.108609	1.588669	-0.631925
17	6	0	1.196087	-0.786496	0.263309
18	7	0	0.680270	-1.937215	0.527952
19	1	0	-0.809194	0.260133	-0.592951
20	7	0	-2.849761	0.530235	0.990550
21	6	0	-2.854101	-0.010144	-0.242577
22	7	0	-3.951350	-0.700037	-0.657960
23	7	0	-1.798095	0.123064	-1.022344
24	6	0	-1.909377	1.593617	1.354657

25	6	0	-3.530475	-0.105406	2.111698
26	6	0	-5.301046	-0.267696	-0.315412
27	6	0	-3.852789	-1.618575	-1.782077
28	1	0	-1.589372	2.139730	0.466413
29	1	0	-1.017552	1.179407	1.834243
30	1	0	-2.426703	2.271708	2.040070
31	1	0	-3.966309	-1.056295	1.804039
32	1	0	-4.315461	0.544115	2.515368
33	1	0	-2.795425	-0.296861	2.900307
34	1	0	-5.848136	-0.032068	-1.235542
35	1	0	-5.841494	-1.054172	0.222500
36	1	0	-4.634742	-2.374806	-1.677325
37	1	0	-2.883651	-2.121285	-1.769976
38	1	0	-3.993601	-1.108471	-2.745340
39	1	0	-5.262831	0.630069	0.301508

TMG-**20**

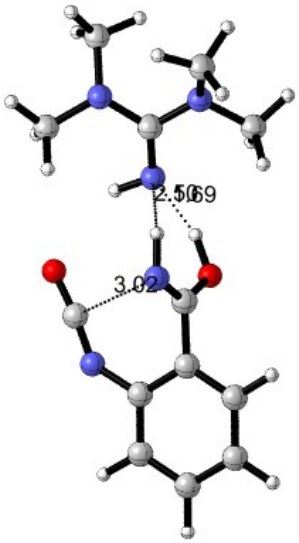
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.640328	0.435834	-2.104589
2	1	0	-0.771740	-1.477799	-0.386820
3	6	0	3.198881	0.441726	-0.017855
4	6	0	4.569006	0.302899	0.231521
5	6	0	5.152175	-0.954385	0.308378
6	6	0	4.366663	-2.095978	0.151551
7	6	0	2.399536	-0.703794	-0.191464
8	6	0	3.005544	-1.960429	-0.090375
9	1	0	4.811627	-3.084003	0.217219
10	1	0	6.218252	-1.041264	0.496759
11	7	0	2.713519	1.748615	-0.026464
12	1	0	2.368596	-2.831138	-0.209098
13	6	0	1.738295	2.424874	-0.222990
14	8	0	0.885516	3.218684	-0.357704
15	8	0	0.560040	0.406340	-1.184706
16	1	0	5.156012	1.205369	0.368564



17	6	0	0.934442	-0.666313	-0.474826
18	7	0	0.187255	-1.617720	-0.061002
19	1	0	-0.452970	0.469389	-1.245660
20	7	0	-2.390384	0.321578	1.066583
21	6	0	-2.840337	0.095000	-0.209519
22	7	0	-4.056149	-0.562957	-0.301306
23	7	0	-2.123703	0.460663	-1.229900
24	6	0	-1.316988	1.274885	1.293782
25	6	0	-2.526319	-0.686355	2.109875
26	6	0	-5.162871	-0.194951	0.572170
27	6	0	-4.464241	-1.084811	-1.590136
28	1	0	-1.317770	2.032214	0.510058
29	1	0	-0.337292	0.777431	1.311897
30	1	0	-1.478403	1.752858	2.265933
31	1	0	-3.212752	-1.471732	1.792650
32	1	0	-2.902235	-0.230395	3.033579
33	1	0	-1.547143	-1.140881	2.310890
34	1	0	-5.894736	0.415236	0.024199
35	1	0	-5.668210	-1.093106	0.944720
36	1	0	-5.249789	-1.828535	-1.430870
37	1	0	-3.621024	-1.577124	-2.080166
38	1	0	-4.864418	-0.302717	-2.254967
39	1	0	-4.796605	0.384717	1.418946

TMG-**TS$_{20/21}$**



Standard orientation:

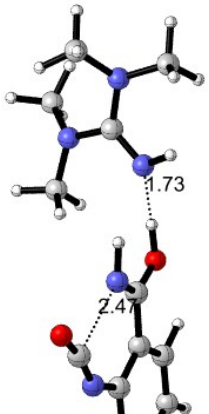
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.500935	1.100285	-0.934401
2	7	0	3.677823	0.884802	0.265385
3	6	0	2.869522	-0.099105	-0.282073
4	7	0	3.375643	-1.382803	-0.226444
5	7	0	1.705279	0.110987	-0.806211
6	6	0	3.097893	2.202561	0.456081
7	6	0	5.102794	0.903298	-0.042921
8	6	0	4.046958	-1.850870	0.979929

9	6	0	2.626368	-2.419447	-0.916441
10	1	0	2.108463	2.119953	0.911484
11	1	0	3.008295	2.763319	-0.487980
12	1	0	3.746398	2.768910	1.129771
13	1	0	5.431583	-0.081108	-0.375243
14	1	0	5.676026	1.192991	0.844467
15	1	0	5.311777	1.626865	-0.844023
16	1	0	3.355636	-2.443800	1.595953
17	1	0	4.901416	-2.482387	0.713489
18	1	0	3.274491	-3.293007	-1.030422
19	1	0	2.320812	-2.062867	-1.900463
20	1	0	1.726876	-2.717212	-0.357025
21	1	0	4.396938	-1.007757	1.574805
22	1	0	0.348732	-0.454729	1.211513
23	6	0	-3.315794	0.710723	-0.036425
24	6	0	-4.698974	0.866238	-0.104361
25	6	0	-5.523863	-0.246313	0.030920
26	6	0	-4.971737	-1.510481	0.230444
27	6	0	-2.750916	-0.555312	0.170054
28	6	0	-3.587586	-1.659141	0.297205
29	1	0	-5.616041	-2.378182	0.333519
30	1	0	-6.601429	-0.122962	-0.021444
31	7	0	-2.506763	1.843831	-0.190080
32	1	0	0.261055	-0.756997	-0.937057
33	1	0	-3.144588	-2.638586	0.453311
34	6	0	-1.342096	2.145130	-0.181607
35	8	0	-0.248312	2.576200	-0.219738
36	8	0	-0.719702	-1.004807	-0.938963
37	1	0	-5.109466	1.858248	-0.262884
38	6	0	-1.261863	-0.667782	0.240114
39	7	0	-0.665985	-0.382406	1.329742

TMG-**21**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

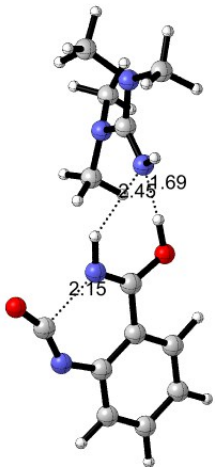


1	1	0	-2.339976	0.189174	-1.859962
2	7	0	-4.476030	0.074399	-0.594005
3	6	0	-3.183612	-0.222076	-0.177644
4	7	0	-3.056128	-0.536168	1.154147
5	7	0	-2.142453	-0.224575	-0.952179
6	6	0	-4.722762	0.177810	-2.019064
7	6	0	-5.291010	0.985428	0.204153
8	6	0	-4.055445	-1.360595	1.821738
9	6	0	-1.714009	-0.684426	1.694827
10	1	0	-4.259901	-0.661736	-2.542709
11	1	0	-4.350263	1.123410	-2.445099
12	1	0	-5.802210	0.133705	-2.186564
13	1	0	-4.943499	1.000184	1.236486
14	1	0	-6.338321	0.666032	0.182371
15	1	0	-5.228134	2.007728	-0.195868
16	1	0	-3.677617	-2.385248	1.942347
17	1	0	-4.277319	-0.954711	2.814960
18	1	0	-1.782750	-0.654067	2.785554
19	1	0	-1.079342	0.138272	1.361580
20	1	0	-1.251598	-1.633495	1.390674
21	1	0	-4.973584	-1.399542	1.236533
22	1	0	-0.554855	-0.894552	-0.814343
23	6	0	3.618591	0.408452	0.083873
24	6	0	2.591467	2.637633	0.321279
25	8	0	0.399910	-1.195138	-0.729789
26	1	0	-0.193619	1.174273	-0.539011
27	6	0	1.188590	-0.142329	-0.465833
28	7	0	0.809684	1.075061	-0.373997
29	6	0	2.615091	-0.517360	-0.278669
30	7	0	3.428043	1.761910	0.321572
31	8	0	1.987393	3.637088	0.398349
32	6	0	2.983504	-1.855720	-0.473942
33	1	0	2.206964	-2.558980	-0.752252
34	6	0	4.295050	-2.285855	-0.324006
35	6	0	4.939109	-0.036408	0.237144
36	1	0	5.686844	0.697860	0.519178
37	6	0	5.279070	-1.365746	0.035556
38	1	0	4.546218	-3.329361	-0.486797
39	1	0	6.310905	-1.681776	0.159194

TMG-**TS$_{21/22}$**

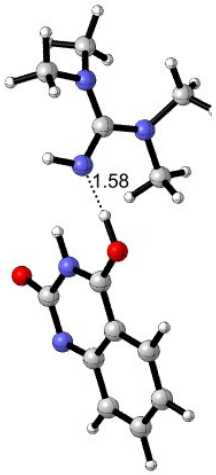
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.292515	0.418855	-1.803628
2	7	0	-4.429554	0.104728	-0.578937
3	6	0	-3.135224	-0.203680	-0.185628
4	7	0	-3.006616	-0.662103	1.101960
5	7	0	-2.089332	-0.092149	-0.948274
6	6	0	-4.676717	0.347579	-1.987039
7	6	0	-5.285581	0.884870	0.309610
8	6	0	-3.993393	-1.569316	1.673558
9	6	0	-1.667075	-0.826943	1.643824
10	1	0	-4.187263	-0.419043	-2.592040
11	1	0	-4.333808	1.343126	-2.311630
12	1	0	-5.754008	0.287330	-2.163210
13	1	0	-4.922670	0.823787	1.335058
14	1	0	-6.313138	0.507722	0.268943
15	1	0	-5.288342	1.941519	0.006897
16	1	0	-3.586174	-2.588837	1.711553
17	1	0	-4.248025	-1.260641	2.693632
18	1	0	-1.746145	-0.891032	2.732401
19	1	0	-1.048855	0.034409	1.387163
20	1	0	-1.181393	-1.737307	1.266524
21	1	0	-4.897877	-1.582721	1.066367
22	1	0	-0.545945	-0.785031	-0.895688
23	6	0	3.592926	0.456970	0.113103
24	6	0	2.346728	2.507606	0.374440
25	8	0	0.410321	-1.109488	-0.848502
26	1	0	-0.138045	1.282284	-0.392444
27	6	0	1.212076	-0.115374	-0.468196
28	7	0	0.853931	1.095493	-0.243725
29	6	0	2.628190	-0.490132	-0.296922
30	7	0	3.357552	1.793429	0.392120
31	8	0	1.737497	3.504141	0.502116
32	6	0	3.022194	-1.812362	-0.543512



33	1	0	2.263801	-2.520208	-0.860552
34	6	0	4.341183	-2.212864	-0.391752
35	6	0	4.924041	0.035512	0.263474
36	1	0	5.651206	0.775768	0.581499
37	6	0	5.295060	-1.276691	0.016170
38	1	0	4.625336	-3.241678	-0.589571
39	1	0	6.333012	-1.572358	0.141027

TMG-**22**

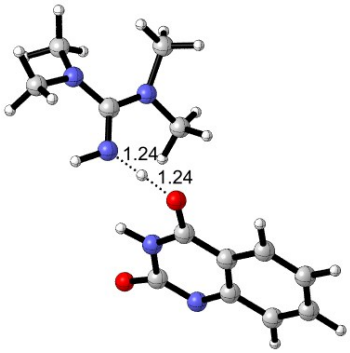


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.171578	0.642141	-1.717701
2	7	0	-4.296296	0.091312	-0.569768
3	6	0	-3.002807	-0.187764	-0.179898
4	7	0	-2.861611	-0.764093	1.052707
5	7	0	-1.952488	0.058061	-0.915356
6	6	0	-4.547989	0.440852	-1.955786
7	6	0	-5.239687	0.683361	0.374436
8	6	0	-3.811483	-1.759029	1.535310
9	6	0	-1.531067	-0.874193	1.631109
10	1	0	-3.988804	-0.222818	-2.619202
11	1	0	-4.288428	1.487229	-2.178805
12	1	0	-5.614062	0.305810	-2.156323
13	1	0	-4.861705	0.594827	1.392284
14	1	0	-6.212308	0.183907	0.305754
15	1	0	-5.376594	1.749385	0.149008
16	1	0	-3.340320	-2.750589	1.533782
17	1	0	-4.124294	-1.525031	2.558900
18	1	0	-1.641265	-1.049143	2.704224
19	1	0	-0.982805	0.058192	1.488766
20	1	0	-0.959104	-1.702428	1.191909
21	1	0	-4.689013	-1.793901	0.890409
22	1	0	-0.547154	-0.655466	-0.958364
23	6	0	3.464764	0.584777	0.180631
24	6	0	1.740852	2.127073	0.342339

25	8	0	0.421393	-1.030550	-0.966795
26	1	0	-0.093666	1.342665	-0.299206
27	6	0	1.278788	-0.152600	-0.510648
28	7	0	0.883021	1.079118	-0.186927
29	6	0	2.644321	-0.466100	-0.336721
30	7	0	3.036880	1.816082	0.503727
31	8	0	1.177460	3.183948	0.586679
32	6	0	3.169487	-1.744706	-0.649524
33	1	0	2.495896	-2.501988	-1.039189
34	6	0	4.502115	-1.999137	-0.458030
35	6	0	4.849116	0.272426	0.362721
36	1	0	5.486614	1.059193	0.753097
37	6	0	5.339480	-0.969079	0.053975
38	1	0	4.919561	-2.972872	-0.692521
39	1	0	6.396328	-1.174931	0.203931

TMG-**TS$_{22/23}$**



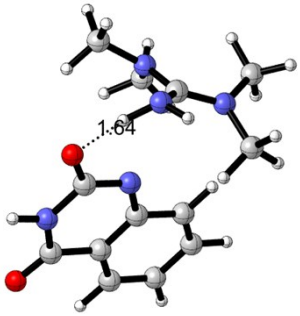
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.313225	0.899720	-1.704645
2	7	0	-4.280813	0.039617	-0.424469
3	6	0	-2.952531	-0.150216	-0.158434
4	7	0	-2.629589	-0.789258	0.990983
5	7	0	-2.009492	0.260889	-0.978302
6	6	0	-4.697835	0.416341	-1.765022
7	6	0	-5.215749	0.409657	0.634305
8	6	0	-3.451937	-1.865214	1.530480
9	6	0	-1.268926	-0.731292	1.516634
10	1	0	-4.125183	-0.141814	-2.508429
11	1	0	-4.586648	1.495502	-1.946068
12	1	0	-5.753429	0.158710	-1.881328
13	1	0	-4.713820	0.400786	1.601507
14	1	0	-6.067001	-0.279204	0.661663
15	1	0	-5.590278	1.423833	0.450844
16	1	0	-2.859392	-2.786578	1.555190

17	1	0	-3.779111	-1.633980	2.550282
18	1	0	-1.320699	-0.877338	2.598611
19	1	0	-0.833701	0.249620	1.320208
20	1	0	-0.630581	-1.505674	1.075951
21	1	0	-4.324507	-2.032046	0.898980
22	1	0	-0.874023	-0.215556	-1.087456
23	6	0	3.412867	0.476496	0.209230
24	6	0	1.881296	2.209622	0.339437
25	8	0	0.272244	-0.684493	-1.204865
26	1	0	0.039872	1.718547	-0.486284
27	6	0	1.193926	0.034310	-0.673800
28	7	0	0.949506	1.305353	-0.307503
29	6	0	2.513098	-0.440126	-0.413296
30	7	0	3.113799	1.739547	0.572719
31	8	0	1.425517	3.315845	0.606580
32	6	0	2.903229	-1.755494	-0.753069
33	1	0	2.172472	-2.404233	-1.228230
34	6	0	4.180544	-2.184302	-0.488518
35	6	0	4.731623	-0.009508	0.464903
36	1	0	5.429055	0.677066	0.934494
37	6	0	5.094470	-1.289217	0.127212
38	1	0	4.492835	-3.190632	-0.748547
39	1	0	6.106950	-1.626930	0.335154

TMG-**23**

Standard orientation:



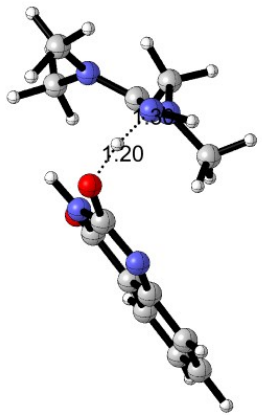
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.801282	-1.852611	-1.064218
2	7	0	2.436799	-0.567802	1.076223
3	6	0	2.527765	-0.191294	-0.211182
4	7	0	2.637277	1.112709	-0.530467
5	7	0	2.579963	-1.139039	-1.154175
6	6	0	2.648386	-1.967321	1.441051
7	6	0	1.610122	0.184346	2.016890
8	6	0	3.226380	2.101535	0.357951

9	6	0	2.227029	1.571852	-1.850709
10	1	0	3.449940	-2.387016	0.832408
11	1	0	1.735242	-2.553240	1.286867
12	1	0	2.939295	-1.996092	2.494261
13	1	0	1.184606	1.063847	1.536095
14	1	0	2.193869	0.474512	2.897366
15	1	0	0.772859	-0.450896	2.325146
16	1	0	3.989186	2.661953	-0.193107
17	1	0	2.472883	2.806603	0.729369
18	1	0	1.904867	2.613247	-1.767708
19	1	0	1.372689	0.976663	-2.184876
20	1	0	3.048685	1.524106	-2.577830
21	1	0	3.701311	1.604020	1.204146
22	1	0	2.768331	-0.824804	-2.096517
23	6	0	-1.276109	0.522439	-0.174500
24	6	0	-0.516574	-1.644061	-0.510219
25	8	0	-4.049153	-1.801248	0.064503
26	1	0	-1.978628	-3.092494	-0.417217
27	6	0	-2.939088	-1.308755	-0.074252
28	7	0	-1.830060	-2.092038	-0.340184
29	6	0	-2.617257	0.121338	0.018830
30	7	0	-0.243552	-0.342592	-0.438487
31	8	0	0.350607	-2.538430	-0.715708
32	6	0	-3.625710	1.052741	0.292550
33	1	0	-4.637345	0.679755	0.427764
34	6	0	-3.327863	2.401775	0.383929
35	6	0	-0.997499	1.907032	-0.076655
36	1	0	0.029278	2.233461	-0.230201
37	6	0	-1.999576	2.820383	0.196441
38	1	0	-4.106995	3.127547	0.593982
39	1	0	-1.756012	3.878141	0.262797

TMG-**TS$_{23/24}$**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.458640	2.063586	0.542138

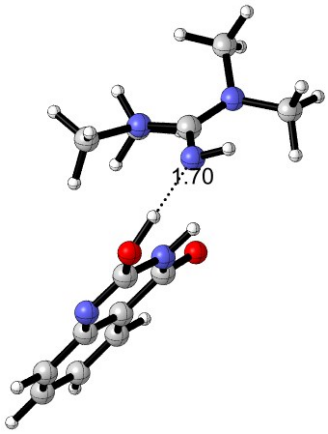


2	7	0	3.103992	-0.037383	-0.256006
3	6	0	2.229245	0.018206	0.784702
4	7	0	1.624520	-1.133206	1.178833
5	7	0	1.990962	1.193418	1.339935
6	6	0	3.974168	1.103882	-0.513094
7	6	0	2.937132	-0.961978	-1.373658
8	6	0	2.258653	-2.440031	1.098010
9	6	0	0.362276	-1.092258	1.901090
10	1	0	4.251484	1.573106	0.430332
11	1	0	3.477419	1.853199	-1.143666
12	1	0	4.870771	0.742613	-1.024473
13	1	0	1.988213	-1.497535	-1.301981
14	1	0	3.767768	-1.675243	-1.429568
15	1	0	2.924652	-0.386840	-2.308061
16	1	0	2.222255	-2.912834	2.086233
17	1	0	1.742835	-3.086908	0.378810
18	1	0	-0.245306	-1.946412	1.585999
19	1	0	-0.186845	-0.178905	1.656912
20	1	0	0.512099	-1.146928	2.988125
21	1	0	3.303806	-2.331875	0.807045
22	1	0	1.497041	1.130498	2.225175
23	6	0	-2.350636	0.883135	0.089783
24	6	0	-0.287171	1.781659	-0.348590
25	8	0	-0.353916	-1.477059	-1.810922
26	1	0	0.899621	0.667841	-1.616258
27	6	0	-0.772668	-0.472026	-1.244273
28	7	0	0.002821	0.668037	-1.142397
29	6	0	-2.080387	-0.314714	-0.607700
30	7	0	-1.430477	1.902645	0.256181
31	8	0	0.707371	2.612148	-0.221071
32	6	0	-3.033174	-1.340919	-0.690108
33	1	0	-2.772536	-2.240936	-1.240033
34	6	0	-4.268307	-1.184858	-0.089754
35	6	0	-3.618037	1.019492	0.695716
36	1	0	-3.826136	1.939962	1.232389
37	6	0	-4.553718	0.006376	0.603461
38	1	0	-5.014978	-1.970047	-0.156012
39	1	0	-5.525415	0.132587	1.073511

TMG-**24**

Standard orientation:

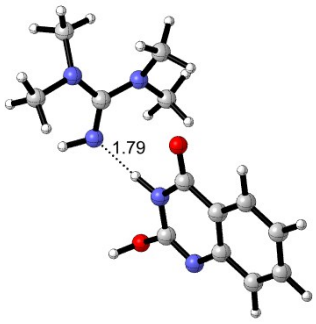
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.971011	2.266096	-0.581910
2	7	0	-2.097328	0.092710	1.260770
3	6	0	-2.758224	0.373388	0.095396
4	7	0	-3.675426	-0.566937	-0.313504
5	7	0	-2.466154	1.453564	-0.579583
6	6	0	-1.419691	1.148152	1.994298
7	6	0	-1.654770	-1.257957	1.584203
8	6	0	-4.522502	-1.275147	0.635136
9	6	0	-4.162539	-0.542890	-1.678398
10	1	0	-1.870792	2.111241	1.755971
11	1	0	-0.347308	1.188222	1.760368
12	1	0	-1.527197	0.949368	3.066109
13	1	0	-1.936538	-1.951785	0.791624
14	1	0	-2.075784	-1.594497	2.539911
15	1	0	-0.560532	-1.269825	1.661163
16	1	0	-5.572997	-1.005914	0.465632
17	1	0	-4.417495	-2.360377	0.520313
18	1	0	-4.547577	-1.535440	-1.926984
19	1	0	-3.344501	-0.313333	-2.365304
20	1	0	-4.973921	0.186876	-1.822018
21	1	0	-4.256031	-0.997126	1.654655
22	1	0	-3.163080	1.670965	-1.287165
23	6	0	2.868342	0.655247	-0.053827
24	6	0	0.834535	1.586967	-0.482112
25	8	0	0.476935	-1.909922	-0.988046
26	1	0	-0.643606	0.289575	-1.132622
27	6	0	1.026134	-0.846625	-0.734851
28	7	0	0.321200	0.346688	-0.816613
29	6	0	2.418469	-0.654125	-0.328038
30	7	0	2.055885	1.774249	-0.113950
31	8	0	-0.014654	2.598131	-0.551448
32	6	0	3.281900	-1.754545	-0.226532
33	1	0	2.885611	-2.741079	-0.450077



34	6	0	4.599560	-1.564520	0.144931
35	6	0	4.215874	0.826726	0.322326
36	1	0	4.560021	1.834545	0.532700
37	6	0	5.060390	-0.263519	0.417737
38	1	0	5.275845	-2.409960	0.223749
39	1	0	6.096535	-0.112061	0.708380

TMG-**TS$_{24/25}$**

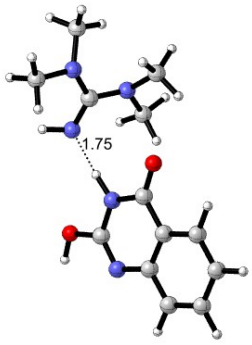
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.824419	3.626009	-0.464107
2	7	0	-2.637353	-0.472336	1.172334
3	6	0	-2.847970	0.272719	0.040651
4	7	0	-3.808322	-0.236150	-0.826804
5	7	0	-2.173378	1.363591	-0.162098
6	6	0	-1.811637	0.081832	2.228614
7	6	0	-2.651277	-1.928655	1.133852
8	6	0	-5.085289	-0.702887	-0.305149
9	6	0	-3.886364	0.321318	-2.159907
10	1	0	-1.949406	1.162283	2.275720
11	1	0	-0.748595	-0.138939	2.060606
12	1	0	-2.115317	-0.369163	3.179160
13	1	0	-3.010076	-2.277483	0.165771
14	1	0	-3.296474	-2.325626	1.927898
15	1	0	-1.631984	-2.306217	1.271661
16	1	0	-5.860017	0.067719	-0.432997
17	1	0	-5.403560	-1.606548	-0.837238
18	1	0	-4.454064	-0.367899	-2.791682
19	1	0	-2.883214	0.425213	-2.579583
20	1	0	-4.395626	1.299547	-2.183484
21	1	0	-4.998778	-0.929025	0.757203
22	1	0	-2.570982	1.912760	-0.919845
23	6	0	3.264282	0.457333	-0.064358
24	6	0	1.572027	1.954045	0.141721
25	8	0	0.044780	-1.201966	-0.247974

26	1	0	-0.400657	1.237728	0.039768
27	6	0	0.926348	-0.356859	-0.159784
28	7	0	0.618357	0.983968	0.016666
29	6	0	2.370129	-0.620833	-0.206967
30	7	0	2.841006	1.769461	0.112379
31	8	0	1.066413	3.196761	0.370009
32	6	0	2.844464	-1.927606	-0.385683
33	1	0	2.117913	-2.727935	-0.491677
34	6	0	4.206256	-2.166188	-0.424280
35	6	0	4.646674	0.197779	-0.103328
36	1	0	5.328184	1.035193	0.009452
37	6	0	5.105548	-1.094719	-0.281500
38	1	0	4.582383	-3.175075	-0.563032
39	1	0	6.174979	-1.284314	-0.310494

TMG-**25**

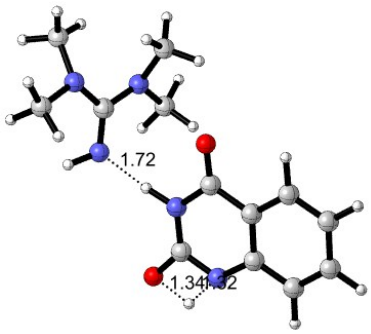


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.757942	3.757225	0.502449
2	7	0	-2.708066	-0.654796	1.091730
3	6	0	-2.876230	0.252590	0.075931
4	7	0	-3.855522	-0.081585	-0.853808
5	7	0	-2.150248	1.326689	0.031372
6	6	0	-1.878342	-0.280909	2.222242
7	6	0	-2.752980	-2.088905	0.836951
8	6	0	-5.150989	-0.567244	-0.399288
9	6	0	-3.913260	0.676898	-2.085278
10	1	0	-2.007656	0.780338	2.436284
11	1	0	-0.817650	-0.484194	2.024508
12	1	0	-2.191723	-0.870730	3.089954
13	1	0	-3.143847	-2.281725	-0.162145
14	1	0	-3.390117	-2.586431	1.578984
15	1	0	-1.739418	-2.501904	0.891584
16	1	0	-5.889098	0.248876	-0.390636
17	1	0	-5.513927	-1.355882	-1.068086

18	1	0	-4.508006	0.114883	-2.811145
19	1	0	-2.907820	0.806622	-2.491912
20	1	0	-4.383240	1.665749	-1.954058
21	1	0	-5.069485	-0.968067	0.610484
22	1	0	-2.507770	2.002352	-0.638933
23	6	0	3.289173	0.490230	-0.059008
24	6	0	1.553178	1.922851	0.236275
25	8	0	0.107160	-1.244978	-0.215917
26	1	0	-0.408862	1.173788	0.166812
27	6	0	0.967267	-0.380468	-0.112916
28	7	0	0.620467	0.942615	0.123677
29	6	0	2.416471	-0.605698	-0.205567
30	7	0	2.832617	1.780770	0.164530
31	8	0	1.014622	3.134234	0.439460
32	6	0	2.916634	-1.894750	-0.434784
33	1	0	2.205672	-2.708753	-0.542773
34	6	0	4.281741	-2.101224	-0.518190
35	6	0	4.675177	0.264350	-0.145877
36	1	0	5.342119	1.113433	-0.032497
37	6	0	5.158224	-1.011881	-0.371839
38	1	0	4.676769	-3.096860	-0.694479
39	1	0	6.230739	-1.173676	-0.437156

TMG-**TS$_{25/26}$**



Standard orientation:

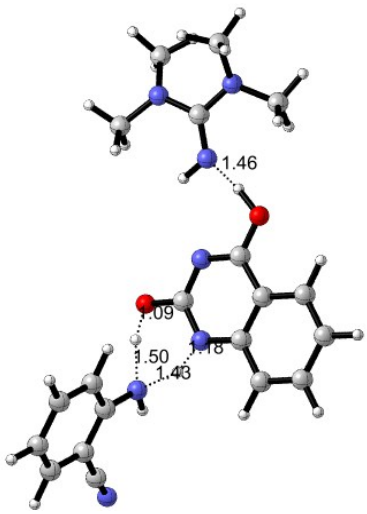
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.670491	3.019024	0.353608
2	7	0	-2.727844	-0.617698	1.098043
3	6	0	-2.900816	0.273020	0.068402
4	7	0	-3.891785	-0.067825	-0.844050
5	7	0	-2.166092	1.339918	-0.003251
6	6	0	-1.895671	-0.227930	2.221288
7	6	0	-2.786438	-2.055299	0.870592
8	6	0	-5.182510	-0.550326	-0.372636
9	6	0	-3.958883	0.670077	-2.087990

10	1	0	-2.014145	0.838864	2.412754
11	1	0	-0.836607	-0.445900	2.030296
12	1	0	-2.215449	-0.795780	3.101253
13	1	0	-3.176867	-2.263381	-0.125664
14	1	0	-3.429406	-2.533886	1.620033
15	1	0	-1.777362	-2.477938	0.936712
16	1	0	-5.926323	0.260042	-0.388713
17	1	0	-5.540533	-1.362708	-1.015301
18	1	0	-4.561339	0.097119	-2.798702
19	1	0	-2.957015	0.791073	-2.505807
20	1	0	-4.425590	1.661614	-1.968369
21	1	0	-5.096524	-0.917864	0.649383
22	1	0	-2.524902	2.011081	-0.677190
23	6	0	3.319459	0.458205	-0.060093
24	6	0	1.513547	1.943139	0.238115
25	8	0	0.086758	-1.208251	-0.218193
26	1	0	-0.455665	1.206647	0.153216
27	6	0	0.946304	-0.348357	-0.112093
28	7	0	0.581344	0.981455	0.125848
29	6	0	2.399494	-0.602059	-0.204263
30	7	0	2.824882	1.723281	0.164265
31	8	0	1.344063	3.197219	0.425891
32	6	0	2.861427	-1.903207	-0.434740
33	1	0	2.125209	-2.694393	-0.542772
34	6	0	4.220302	-2.155466	-0.521012
35	6	0	4.695572	0.197874	-0.147549
36	1	0	5.395667	1.019579	-0.034643
37	6	0	5.131114	-1.096727	-0.375643
38	1	0	4.581257	-3.163192	-0.699173
39	1	0	6.197595	-1.293317	-0.442770

TMG-**TS$_{25/26}$'**

Standard orientation:

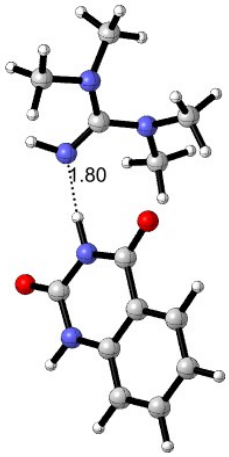
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843937	2.208913	-0.058148



2	6	0	-1.765803	3.255236	-0.259519
3	6	0	-1.338048	4.481627	-0.736055
4	6	0	0.016907	4.711384	-1.029091
5	6	0	0.511468	2.446823	-0.354626
6	6	0	0.932969	3.692061	-0.836886
7	1	0	0.339406	5.678504	-1.401284
8	1	0	-2.063474	5.277067	-0.884045
9	7	0	-1.286982	0.991547	0.414453
10	1	0	1.989826	3.824808	-1.050240
11	6	0	-0.404106	0.002378	0.604065
12	8	0	-0.764949	-1.145831	1.021138
13	8	0	2.684666	1.452244	-0.366477
14	1	0	-2.813563	3.077412	-0.032840
15	6	0	1.483166	1.363268	-0.146622
16	7	0	0.931673	0.192672	0.343216
17	1	0	-2.649035	0.399186	0.856887
18	1	0	-2.189749	-1.062841	1.255675
19	7	0	-3.194120	-0.540254	1.171406
20	6	0	-4.002077	-1.066746	0.115376
21	6	0	-5.376956	-1.280967	0.279344
22	6	0	-6.142401	-1.784966	-0.779228
23	6	0	-5.535222	-2.067968	-1.995147
24	6	0	-3.397072	-1.353438	-1.106206
25	6	0	-4.165143	-1.850650	-2.153816
26	1	0	-3.682900	-0.441849	2.062502
27	6	0	-5.980972	-0.978442	1.548055
28	1	0	-7.205153	-1.947276	-0.631718
29	1	0	-3.687522	-2.071683	-3.103296
30	1	0	-6.126706	-2.457605	-2.816998
31	1	0	-2.329060	-1.189673	-1.218126
32	7	0	-6.412456	-0.718698	2.591100
33	1	0	1.581113	-0.613262	0.484028
34	1	0	2.733851	-2.687209	-0.135387
35	7	0	5.008612	-1.885471	-0.769510
36	6	0	4.148334	-1.439415	0.234714
37	7	0	4.684616	-0.489037	1.069851
38	7	0	2.934544	-1.853616	0.411426
39	6	0	4.440325	-2.684233	-1.833730
40	6	0	6.373590	-2.257864	-0.425183
41	6	0	5.530828	0.576618	0.548550

42	6	0	3.933383	-0.119356	2.254782
43	1	0	3.512750	-2.228076	-2.187276
44	1	0	4.239191	-3.724623	-1.526002
45	1	0	5.150478	-2.710867	-2.665452
46	1	0	6.694646	-1.727013	0.470480
47	1	0	7.049028	-2.005147	-1.250136
48	1	0	6.447714	-3.339526	-0.233179
49	1	0	4.972718	1.519782	0.545756
50	1	0	6.429867	0.685330	1.168582
51	1	0	4.631397	0.296866	2.988688
52	1	0	3.446972	-1.001861	2.670920
53	1	0	3.170461	0.636989	2.025808
54	1	0	5.823395	0.355681	-0.478020

TMG-**26**



Standard orientation:

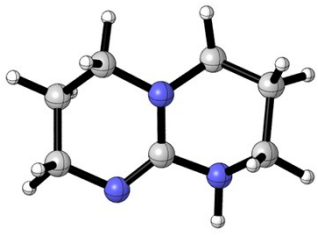
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.316026	0.442906	-0.067475
2	6	0	4.687773	0.172832	-0.158427
3	6	0	5.112858	-1.129267	-0.376860
4	6	0	4.192704	-2.177502	-0.508077
5	6	0	2.391605	-0.600992	-0.196172
6	6	0	2.835927	-1.906688	-0.416913
7	1	0	4.541202	-3.190666	-0.679021
8	1	0	6.177592	-1.332862	-0.446424
9	7	0	2.846792	1.727684	0.149232
10	1	0	2.087327	-2.687369	-0.513739
11	6	0	1.510639	2.076900	0.242338
12	8	0	1.158364	3.228136	0.406484
13	8	0	0.075639	-1.158850	-0.190417
14	1	0	5.406688	0.981462	-0.057090
15	6	0	0.945682	-0.306486	-0.093794
16	7	0	0.627705	1.017961	0.138407
17	1	0	3.492325	2.503417	0.224833
18	1	0	-0.395737	1.248059	0.178216

19	1	0	-2.528942	1.992760	-0.687802
20	7	0	-3.854791	-0.115936	-0.870818
21	6	0	-2.894771	0.260364	0.067559
22	7	0	-2.737950	-0.617122	1.114393
23	7	0	-2.180949	1.338505	0.008403
24	6	0	-3.903123	0.620418	-2.116280
25	6	0	-5.159922	-0.573347	-0.413264
26	6	0	-2.756076	-2.057268	0.897088
27	6	0	-1.923562	-0.200509	2.240597
28	1	0	-2.894111	0.746979	-2.515016
29	1	0	-4.377427	1.610106	-2.007234
30	1	0	-4.489160	0.043631	-2.837667
31	1	0	-5.084835	-0.981414	0.594111
32	1	0	-5.540315	-1.350323	-1.085654
33	1	0	-5.881405	0.257930	-0.398246
34	1	0	-1.735561	-2.452807	0.960951
35	1	0	-3.382318	-2.546425	1.653890
36	1	0	-2.228999	-0.778248	3.119241
37	1	0	-2.075628	0.862252	2.430351
38	1	0	-0.856664	-0.382973	2.053769
39	1	0	-3.146268	-2.283609	-0.095245

4.3 TBD-catalyzed reaction

TBD

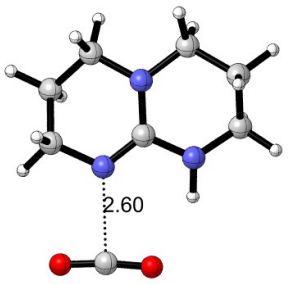
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.161863	1.318590	-0.405034
2	6	0	2.486363	0.697133	0.063909
3	6	0	2.290639	-0.797122	0.363269
4	7	0	0.018949	0.630860	0.193282
5	6	0	-0.078890	-0.728355	-0.068674
6	7	0	1.152932	-1.293674	-0.407877

7	6	0	-1.230050	1.373394	0.377377
8	6	0	-2.389828	0.655154	-0.302631
9	6	0	-2.405199	-0.799048	0.164336
10	7	0	-1.127801	-1.463823	-0.025813
11	1	0	1.059254	-2.303714	-0.432213
12	1	0	1.097679	1.274737	-1.502589
13	1	0	1.111139	2.369480	-0.109570
14	1	0	2.845949	1.202581	0.965773
15	1	0	3.237653	0.840391	-0.719171
16	1	0	2.127485	-0.942021	1.441624
17	1	0	-1.435158	1.482918	1.450877
18	1	0	-1.095489	2.377578	-0.036797
19	1	0	-2.250892	0.686953	-1.390738
20	1	0	-3.334473	1.156711	-0.066794
21	1	0	-2.686606	-0.839280	1.227815
22	1	0	-3.168885	-1.365414	-0.379669
23	1	0	3.174392	-1.372938	0.078985

TBD-**1**

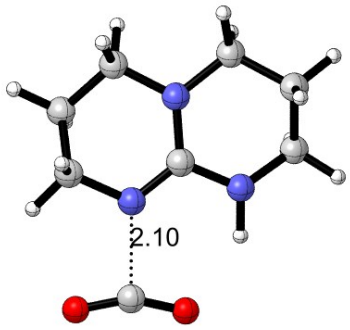


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.659522	-1.900698	0.176632
2	6	0	3.142360	-0.839500	0.109043
3	8	0	3.744062	0.154437	0.072476
4	6	0	-2.764512	0.033115	0.128268
5	6	0	-2.804614	-1.440340	-0.248653
6	6	0	-1.575229	-2.122214	0.332031
7	7	0	-1.448004	0.623915	-0.071975
8	6	0	-0.281493	-0.098938	-0.209314
9	7	0	-0.414421	-1.475667	-0.245048
10	6	0	-1.399686	2.071415	0.105392
11	6	0	0.000821	2.533779	0.479236
12	6	0	1.003588	1.845033	-0.441074
13	7	0	0.900697	0.401645	-0.355038
14	1	0	0.483337	-1.937627	-0.155622

15	1	0	-3.055718	0.153823	1.184933
16	1	0	-3.487736	0.602782	-0.470464
17	1	0	-2.789508	-1.555619	-1.337551
18	1	0	-3.726997	-1.887026	0.135208
19	1	0	-1.546862	-3.180745	0.060634
20	1	0	-1.734545	2.563817	-0.819749
21	1	0	-2.117270	2.338097	0.893218
22	1	0	0.218947	2.254486	1.517045
23	1	0	0.062006	3.624298	0.401983
24	1	0	0.834328	2.177397	-1.478703
25	1	0	2.028748	2.128494	-0.182197
26	1	0	-1.592712	-2.055443	1.433251

TBD-$\mathbf{TS_{1/2}}$

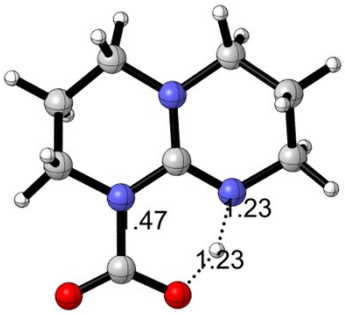


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.276112	-2.034523	0.165498
2	6	0	2.712648	-0.936955	0.049181
3	8	0	3.552407	-0.112901	0.008047
4	6	0	-2.685329	0.294460	0.050603
5	6	0	-2.870127	-1.165399	-0.333510
6	6	0	-1.784325	-1.983254	0.348357
7	7	0	-1.295420	0.724886	-0.052557
8	6	0	-0.228287	-0.135529	-0.128367
9	7	0	-0.506705	-1.474809	-0.103586
10	6	0	-1.095302	2.164448	0.091399
11	6	0	0.341736	2.485599	0.470017
12	6	0	1.269330	1.664377	-0.417924
13	7	0	1.010514	0.247252	-0.263483
14	1	0	0.321664	-2.054561	-0.022896
15	1	0	-3.033535	0.457128	1.082894
16	1	0	-3.287573	0.942877	-0.598891
17	1	0	-2.779060	-1.288226	-1.417969
18	1	0	-3.867674	-1.496824	-0.029905
19	1	0	-1.847223	-3.037416	0.067585

20	1	0	-1.365922	2.661857	-0.851565
21	1	0	-1.791293	2.523434	0.861206
22	1	0	0.522445	2.220570	1.518276
23	1	0	0.520678	3.559328	0.355374
24	1	0	1.133053	1.962721	-1.469835
25	1	0	2.318553	1.838500	-0.166877
26	1	0	-1.893046	-1.917777	1.443090

TBD-**2**

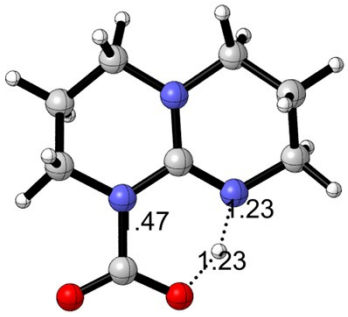


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.835930	-2.133927	-0.127510
2	6	0	-2.244610	-0.972269	0.034930
3	8	0	-3.347510	-0.475160	0.173900
4	6	0	2.560037	0.545728	0.052842
5	6	0	2.858406	-0.880201	0.484658
6	6	0	1.992747	-1.820553	-0.339015
7	7	0	1.124079	0.820371	0.031641
8	6	0	0.198086	-0.174555	-0.027240
9	7	0	0.606250	-1.437191	-0.175578
10	6	0	0.782186	2.240124	-0.041969
11	6	0	-0.661409	2.427397	-0.468485
12	6	0	-1.527252	1.473598	0.334557
13	7	0	-1.112507	0.097839	0.078327
14	1	0	-0.192055	-2.102045	-0.197432
15	1	0	2.978596	0.739363	-0.945659
16	1	0	3.016696	1.262905	0.745051
17	1	0	2.626656	-1.008702	1.547552
18	1	0	3.920994	-1.092052	0.336412
19	1	0	2.093787	-2.854966	-0.003218
20	1	0	0.958037	2.697744	0.941512
21	1	0	1.472016	2.709417	-0.754536
22	1	0	-0.775696	2.210573	-1.536526
23	1	0	-0.963896	3.464566	-0.297838
24	1	0	-1.448543	1.693655	1.409006

25	1	0	-2.579096	1.529827	0.059697
26	1	0	2.286125	-1.780328	-1.397532

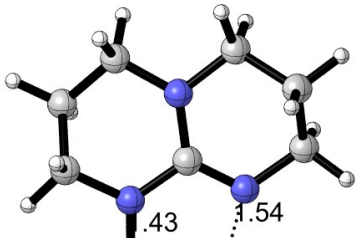
TBD-**$TS_{2/3}$**



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.723051	-2.128293	-0.120979
2	6	0	-2.162813	-0.935840	0.043558
3	8	0	-3.307984	-0.558939	0.186674
4	6	0	2.552999	0.551693	0.046802
5	6	0	2.830315	-0.877554	0.486789
6	6	0	1.953651	-1.819814	-0.328533
7	7	0	1.119250	0.834239	0.018471
8	6	0	0.214658	-0.180156	-0.044662
9	7	0	0.564560	-1.436227	-0.192516
10	6	0	0.763845	2.249566	-0.013329
11	6	0	-0.674367	2.436254	-0.460587
12	6	0	-1.557733	1.475992	0.314984
13	7	0	-1.122541	0.106577	0.060065
14	1	0	-0.501467	-2.055372	-0.188849
15	1	0	2.978900	0.738451	-0.949832
16	1	0	3.012766	1.265943	0.740318
17	1	0	2.593881	-0.992164	1.550625
18	1	0	3.891657	-1.103222	0.347262
19	1	0	2.055422	-2.851611	0.017072
20	1	0	0.916312	2.681544	0.986289
21	1	0	1.457845	2.751072	-0.699501
22	1	0	-0.768202	2.231471	-1.533081
23	1	0	-0.983530	3.470391	-0.283380
24	1	0	-1.511362	1.691518	1.392007
25	1	0	-2.601241	1.532928	0.009041
26	1	0	2.255087	-1.796055	-1.385801

TBD-**3**



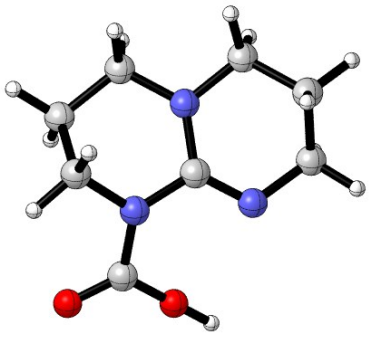
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.837087	-2.107574	-0.152626
2	6	0	-2.182668	-0.857851	0.045728
3	8	0	-3.323564	-0.483723	0.193330
4	6	0	2.565606	0.542859	0.081832
5	6	0	2.844934	-0.891076	0.498765
6	6	0	1.969400	-1.810892	-0.342864
7	7	0	1.130768	0.809733	0.007770
8	6	0	0.235530	-0.226992	-0.041673
9	7	0	0.570119	-1.471731	-0.178395
10	6	0	0.793120	2.225103	-0.081892
11	6	0	-0.658647	2.417296	-0.472636
12	6	0	-1.505349	1.479734	0.366372
13	7	0	-1.117977	0.098491	0.081308
14	1	0	-0.810698	-2.159118	-0.204223
15	1	0	3.021564	0.753354	-0.896992
16	1	0	2.995538	1.250757	0.801792
17	1	0	2.600214	-1.029520	1.558026
18	1	0	3.908203	-1.111678	0.363690
19	1	0	2.101858	-2.856110	-0.051321
20	1	0	0.991106	2.701175	0.890194
21	1	0	1.466657	2.686910	-0.815882
22	1	0	-0.807106	2.188902	-1.533966
23	1	0	-0.952758	3.457215	-0.303237
24	1	0	-1.371662	1.692438	1.436606
25	1	0	-2.565581	1.563361	0.135860
26	1	0	2.255951	-1.731850	-1.402748

TBD-**$TS_{3/4}$**

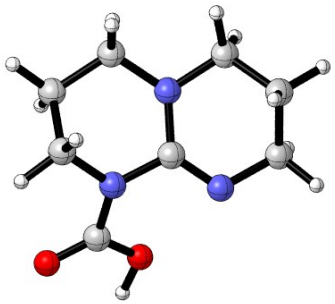
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	8	0	-1.825344	-1.987176	-0.484447
2	6	0	-2.162290	-0.824977	-0.016419
3	8	0	-3.307387	-0.454105	0.112803
4	6	0	2.527441	0.675342	-0.136074
5	6	0	2.974960	-0.650631	0.455156
6	6	0	2.102966	-1.750103	-0.139237
7	7	0	1.074867	0.800759	-0.119230
8	6	0	0.282896	-0.316634	0.099253
9	7	0	0.697987	-1.526733	0.151595
10	6	0	0.613942	2.150165	-0.430077
11	6	0	-0.900455	2.288567	-0.364071
12	6	0	-1.394693	1.361003	0.732852
13	7	0	-1.081005	-0.007742	0.329862
14	1	0	-1.578512	-2.838846	-0.827254
15	1	0	2.887878	0.771636	-1.172137
16	1	0	2.946025	1.518681	0.430326
17	1	0	2.844285	-0.640469	1.543478
18	1	0	4.036881	-0.810570	0.242639
19	1	0	2.380702	-2.728628	0.263775
20	1	0	1.072308	2.828573	0.305255
21	1	0	0.999968	2.441956	-1.417756
22	1	0	-1.371941	1.992061	-1.307245
23	1	0	-1.166563	3.331574	-0.166436
24	1	0	-0.892519	1.578711	1.684082
25	1	0	-2.470665	1.421359	0.879420
26	1	0	2.262453	-1.796167	-1.228886

TBD-**4**



Standard orientation:

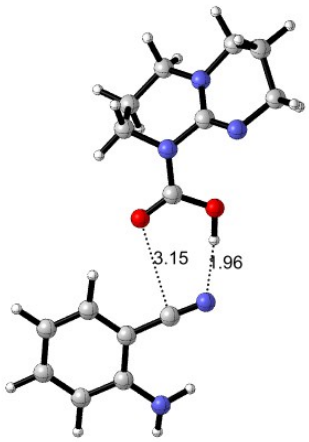
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.754594	-1.895688	-0.748842
2	6	0	-2.117227	-0.814278	-0.043534
3	8	0	-3.283554	-0.545750	0.179402
4	6	0	2.512483	0.634758	-0.335937

5	6	0	2.999379	-0.597800	0.411636
6	6	0	2.108138	-1.779039	0.042627
7	7	0	1.062065	0.773879	-0.242444
8	6	0	0.301033	-0.317346	0.142104
9	7	0	0.712969	-1.507508	0.333370
10	6	0	0.591294	2.145962	-0.407343
11	6	0	-0.919105	2.286783	-0.282327
12	6	0	-1.392484	1.335337	0.805578
13	7	0	-1.070575	-0.017291	0.359896
14	1	0	-2.587243	-2.347729	-0.962604
15	1	0	2.804877	0.583617	-1.395024
16	1	0	2.966818	1.542797	0.082035
17	1	0	2.933222	-0.425193	1.492442
18	1	0	4.048467	-0.789309	0.164461
19	1	0	2.401477	-2.675219	0.597000
20	1	0	1.073842	2.760781	0.369346
21	1	0	0.943839	2.522791	-1.377002
22	1	0	-1.421654	2.020541	-1.218608
23	1	0	-1.168072	3.326703	-0.048470
24	1	0	-0.878252	1.531931	1.754653
25	1	0	-2.467258	1.384221	0.971629
26	1	0	2.222853	-2.014253	-1.026915

TBD-**5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.406618	0.511597	-0.355831
2	6	0	-0.637098	-0.117612	-0.253704
3	8	0	-0.691636	-1.393544	0.109187
4	6	0	-5.390075	-0.023122	0.583561
5	6	0	-5.692626	-1.050951	-0.496345
6	6	0	-4.525364	-2.028821	-0.582275
7	7	0	-4.031367	0.493413	0.456176
8	6	0	-3.105120	-0.209593	-0.298503
9	7	0	-3.272200	-1.347578	-0.845336

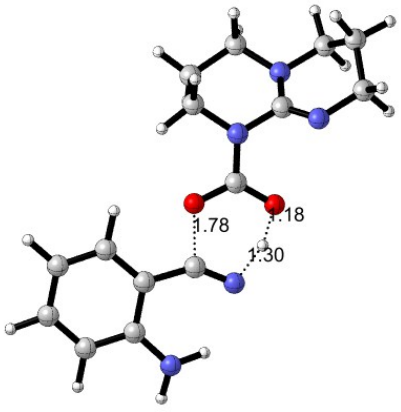


10	6	0	-3.846812	1.815587	1.045122
11	6	0	-2.437586	2.368930	0.871034
12	6	0	-1.920696	1.925336	-0.489770
13	7	0	-1.868092	0.467645	-0.472410
14	1	0	-5.519750	-0.465312	1.582420
15	1	0	-6.083479	0.825535	0.512722
16	1	0	-5.808691	-0.547983	-1.463735
17	1	0	-6.633161	-1.562223	-0.267017
18	1	0	-4.688287	-2.759862	-1.379639
19	1	0	-4.561521	2.499116	0.559184
20	1	0	-4.122522	1.770629	2.107867
21	1	0	-1.759720	1.980396	1.639064
22	1	0	-2.462677	3.459530	0.963820
23	1	0	-2.594343	2.246024	-1.293796
24	1	0	-0.918642	2.294364	-0.700444
25	1	0	-4.443645	-2.597067	0.357287
26	1	0	0.228808	-1.702334	0.245472
27	6	0	5.277204	-0.671589	0.264398
28	6	0	6.262903	0.296097	0.013325
29	6	0	5.912362	1.557268	-0.445207
30	6	0	3.932589	-0.311369	0.034129
31	6	0	3.583585	0.964755	-0.429729
32	6	0	4.575434	1.902475	-0.672094
33	6	0	2.912795	-1.281111	0.297150
34	7	0	5.615393	-1.947089	0.665240
35	1	0	7.306820	0.041287	0.176189
36	1	0	6.696551	2.286186	-0.629966
37	1	0	4.314987	2.891959	-1.031723
38	7	0	2.125225	-2.098230	0.533273
39	1	0	2.531301	1.183850	-0.584312
40	1	0	4.886947	-2.519957	1.073427
41	1	0	6.519487	-2.063365	1.101178

TBD-**$TS_{5/6}$**

Standard orientation:

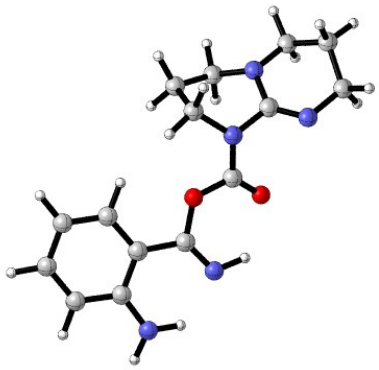
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	8	0	0.766569	0.103332	-0.234549
2	6	0	-0.388092	-0.444155	-0.119850
3	8	0	-0.567035	-1.636086	0.289567
4	6	0	-4.903218	-0.007406	0.891611
5	6	0	-5.475279	-0.647187	-0.367619
6	6	0	-4.492204	-1.709222	-0.847272
7	7	0	-3.551790	0.506725	0.652396
8	6	0	-2.796458	-0.192824	-0.288129
9	7	0	-3.131826	-1.212459	-0.964906
10	6	0	-3.412823	1.960773	0.773887
11	6	0	-1.968490	2.419566	0.631172
12	6	0	-1.356191	1.765526	-0.600751
13	7	0	-1.470180	0.319410	-0.445029
14	1	0	-4.861010	-0.747786	1.700689
15	1	0	-5.526943	0.822928	1.236225
16	1	0	-5.601574	0.119210	-1.143287
17	1	0	-6.458059	-1.083926	-0.162918
18	1	0	-4.784406	-2.099124	-1.827406
19	1	0	-4.033522	2.458845	0.007376
20	1	0	-3.807420	2.249877	1.753075
21	1	0	-1.388669	2.125034	1.513138
22	1	0	-1.940542	3.511364	0.551010
23	1	0	-1.895312	2.059277	-1.510457
24	1	0	-0.303938	2.015580	-0.727833
25	1	0	-4.490495	-2.565213	-0.158494
26	1	0	0.521965	-2.059908	0.468573
27	6	0	4.565608	-0.743796	0.189458
28	6	0	5.724405	0.043270	0.036017
29	6	0	5.640558	1.382487	-0.299495
30	6	0	3.306338	-0.118904	-0.010501
31	6	0	3.245263	1.238436	-0.353288
32	6	0	4.397711	1.993310	-0.499752
33	6	0	2.134641	-0.958195	0.191275
34	7	0	4.676728	-2.076637	0.479418
35	1	0	6.694342	-0.426155	0.180238
36	1	0	6.554885	1.959460	-0.408725
37	1	0	4.333975	3.043005	-0.765828
38	7	0	1.817376	-2.066245	0.535853
39	1	0	2.273078	1.689304	-0.501073

40	1	0	3.844139	-2.582998	0.759515
41	1	0	5.560465	-2.412387	0.831347

TBD-**6**



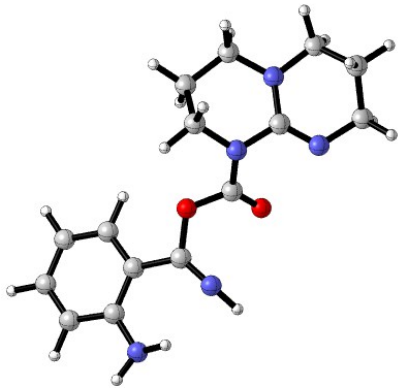
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.767849	-0.331959	-0.291928
2	6	0	-0.484877	-0.818108	-0.032443
3	8	0	-0.715738	-1.819903	0.599626
4	6	0	-4.758008	0.660718	0.782338
5	6	0	-5.519771	-0.242642	-0.177598
6	6	0	-4.734930	-1.536705	-0.387413
7	7	0	-3.411035	0.873986	0.269185
8	6	0	-2.803657	-0.229643	-0.329055
9	7	0	-3.330840	-1.317155	-0.708791
10	6	0	-2.539592	1.745815	1.056302
11	6	0	-1.435669	2.355442	0.173478
12	6	0	-1.141245	1.399501	-0.992339
13	7	0	-1.420347	0.021678	-0.580324
14	1	0	-4.717157	0.201553	1.784393
15	1	0	-5.244507	1.637153	0.881467
16	1	0	-5.639341	0.275968	-1.136198
17	1	0	-6.519212	-0.452350	0.217097
18	1	0	-5.173952	-2.121222	-1.201830
19	1	0	-3.167683	2.528912	1.490080
20	1	0	-2.093795	1.185214	1.892673
21	1	0	-0.536779	2.515641	0.778549
22	1	0	-1.747023	3.326552	-0.224467
23	1	0	-1.804208	1.611911	-1.835096
24	1	0	-0.115013	1.468328	-1.347601
25	1	0	-4.784940	-2.166779	0.510932
26	1	0	1.080293	-2.722839	0.283817
27	6	0	4.421318	-0.650557	0.115943
28	6	0	5.496128	0.266051	0.085760
29	6	0	5.288454	1.620999	-0.079891

30	6	0	3.102329	-0.139761	-0.030673
31	6	0	2.925859	1.244422	-0.198352
32	6	0	3.991320	2.127678	-0.224110
33	6	0	1.933387	-1.039421	0.011804
34	7	0	4.689873	-1.980080	0.249876
35	1	0	6.505922	-0.122877	0.192951
36	1	0	6.142770	2.292186	-0.096605
37	1	0	3.820699	3.191221	-0.352802
38	7	0	1.997112	-2.279994	0.259808
39	1	0	1.917027	1.626861	-0.302962
40	1	0	3.917110	-2.613719	0.423092
41	1	0	5.623293	-2.258612	0.510154

TBD-**TS$_{6/7}$**

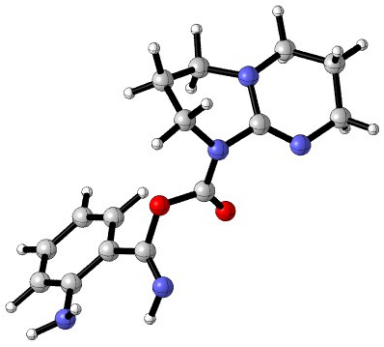
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.813358	-0.080815	0.206830
2	6	0	0.394368	-0.588741	-0.215700
3	8	0	0.499823	-1.366222	-1.122979
4	6	0	4.961929	0.633186	-0.420422
5	6	0	5.452872	-0.730213	0.045639
6	6	0	4.465504	-1.796144	-0.418519
7	7	0	3.540681	0.808453	-0.135831
8	6	0	2.762332	-0.308739	0.124092
9	7	0	3.119429	-1.527425	0.051047
10	6	0	3.141431	2.199546	0.051819
11	6	0	1.661735	2.371445	0.372411
12	6	0	1.236242	1.218251	1.270609
13	7	0	1.423119	-0.016361	0.511368
14	1	0	5.135018	0.756815	-1.499405
15	1	0	5.511738	1.434574	0.090315
16	1	0	5.508837	-0.747384	1.140730
17	1	0	6.458568	-0.913702	-0.345994
18	1	0	4.762002	-2.783990	-0.053643
19	1	0	3.735887	2.612158	0.883448

20	1	0	3.415418	2.767158	-0.847626
21	1	0	1.054331	2.345250	-0.539602
22	1	0	1.506597	3.342743	0.853267
23	1	0	1.866597	1.167850	2.166856
24	1	0	0.198048	1.289166	1.585488
25	1	0	4.460595	-1.851785	-1.517653
26	1	0	-1.806197	-3.108798	0.064973
27	6	0	-4.448740	-0.662045	0.143156
28	6	0	-5.571217	0.168884	-0.042478
29	6	0	-5.433564	1.491350	-0.421578
30	6	0	-3.159009	-0.109456	-0.058044
31	6	0	-3.050181	1.239983	-0.437684
32	6	0	-4.163400	2.040816	-0.627411
33	6	0	-1.940379	-0.932536	0.130511
34	7	0	-4.654753	-1.982683	0.478295
35	1	0	-6.560558	-0.256755	0.107992
36	1	0	-6.322436	2.100710	-0.561266
37	1	0	-4.049927	3.076324	-0.930590
38	7	0	-1.825175	-2.145429	0.320113
39	1	0	-2.058532	1.650123	-0.589428
40	1	0	-3.853712	-2.481204	0.842466
41	1	0	-5.536635	-2.192355	0.925496

TBD-**7**



Standard orientation:

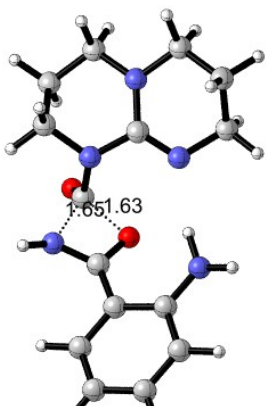
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.791682	-0.728007	0.754795
2	6	0	0.310800	-0.813495	-0.060656
3	8	0	0.234556	-0.990916	-1.248021
4	6	0	4.450875	1.179887	-0.436001
5	6	0	5.281327	-0.053388	-0.762138
6	6	0	4.395939	-1.088071	-1.454019
7	7	0	3.296090	0.784253	0.358959
8	6	0	2.693268	-0.425520	-0.000642
9	7	0	3.143228	-1.338373	-0.754929

10	6	0	2.387976	1.859651	0.755847
11	6	0	1.577639	1.461101	2.001886
12	6	0	1.437737	-0.067244	2.039900
13	7	0	1.449554	-0.596957	0.674724
14	1	0	4.124219	1.672937	-1.367606
15	1	0	5.029643	1.908804	0.142247
16	1	0	5.679804	-0.471450	0.169857
17	1	0	6.130520	0.221858	-1.396143
18	1	0	4.921926	-2.043791	-1.542090
19	1	0	2.997236	2.746190	0.953883
20	1	0	1.710292	2.110185	-0.076268
21	1	0	0.591148	1.934819	1.959467
22	1	0	2.073916	1.803608	2.915781
23	1	0	2.290949	-0.515146	2.556246
24	1	0	0.527246	-0.390783	2.539363
25	1	0	4.159731	-0.767941	-2.478078
26	1	0	-3.064008	-2.660146	-0.244364
27	6	0	-4.311541	-0.228975	0.064321
28	6	0	-5.153086	0.812107	-0.353894
29	6	0	-4.636572	1.944702	-0.966665
30	6	0	-2.924243	-0.102872	-0.152815
31	6	0	-2.418870	1.057044	-0.751035
32	6	0	-3.261284	2.077804	-1.168456
33	6	0	-1.991574	-1.191987	0.222706
34	7	0	-4.862132	-1.376790	0.640300
35	1	0	-6.224253	0.720649	-0.189891
36	1	0	-5.313367	2.732912	-1.284192
37	1	0	-2.855336	2.963225	-1.646181
38	7	0	-2.157831	-2.441336	0.175618
39	1	0	-1.347676	1.130973	-0.914539
40	1	0	-4.280754	-1.837132	1.333629
41	1	0	-5.806933	-1.248422	0.981953

TBD-**$TS_{7/8}$**

Standard orientation:

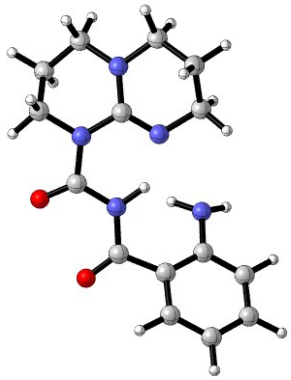
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	6	0	-3.895573	-1.141958	-0.318823
2	6	0	-5.113315	-0.584909	-0.651103
3	6	0	-5.237268	0.811950	-0.610727
4	6	0	-2.809566	-0.340181	0.063273
5	6	0	-2.917908	1.076110	0.091579
6	6	0	-4.177876	1.620170	-0.255061
7	6	0	-1.546466	-0.965484	0.395201
8	7	0	-1.883817	1.890241	0.412466
9	1	0	-2.006547	2.873820	0.238121
10	1	0	-3.763034	-2.220767	-0.315893
11	1	0	-5.954556	-1.208808	-0.927337
12	1	0	-6.186413	1.274194	-0.865706
13	1	0	-4.297313	2.699663	-0.238273
14	8	0	0.901378	-2.264919	1.550711
15	6	0	0.398474	-1.562782	0.712080
16	8	0	-0.684972	-0.449054	1.203687
17	6	0	3.860859	1.667598	-0.376947
18	6	0	2.894493	2.840209	-0.366433
19	6	0	1.824964	2.546993	0.679530
20	7	0	3.158347	0.391452	-0.315701
21	6	0	1.802788	0.338210	-0.054984
22	7	0	1.096071	1.339739	0.338577
23	6	0	4.049093	-0.754348	-0.455917
24	6	0	3.307746	-2.076632	-0.364279
25	6	0	1.970991	-1.880778	-1.062511
26	7	0	1.170243	-0.890530	-0.339979
27	1	0	4.546311	1.736711	0.480923
28	1	0	4.481596	1.675261	-1.283494
29	1	0	2.412653	2.942686	-1.344148
30	1	0	3.439652	3.764829	-0.156965
31	1	0	1.110945	3.373887	0.749783
32	1	0	4.544264	-0.673561	-1.435585
33	1	0	4.837402	-0.685267	0.306711
34	1	0	3.105825	-2.354654	0.672661
35	1	0	3.903396	-2.865131	-0.832584
36	1	0	2.115336	-1.534949	-2.093448
37	1	0	1.397825	-2.810565	-1.096930
38	1	0	2.297252	2.450652	1.669155
39	1	0	-1.196012	-2.512462	-0.929209

40	7	0	-0.979287	-2.063441	-0.048784
41	1	0	-0.919354	1.549012	0.491713

TBD-**8**



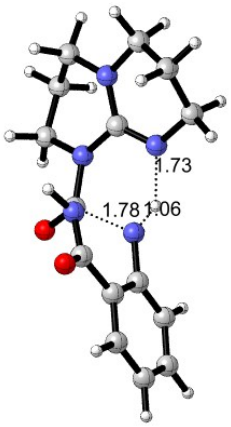
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.556173	-2.997137	0.038923
2	6	0	0.558816	-1.790599	-0.023650
3	6	0	3.586150	2.155609	-0.309235
4	6	0	2.423758	2.887232	-0.959003
5	6	0	1.150983	2.507674	-0.212755
6	7	0	3.279161	0.746044	-0.083815
7	6	0	1.976949	0.302649	-0.152289
8	7	0	0.951697	1.074829	-0.253916
9	6	0	4.435549	-0.041477	0.322110
10	6	0	4.032612	-1.439037	0.749095
11	6	0	2.987455	-1.939624	-0.229098
12	7	0	1.800061	-1.090578	-0.129338
13	1	0	3.840854	2.626586	0.651890
14	1	0	4.482991	2.204700	-0.940127
15	1	0	2.326948	2.582331	-2.005927
16	1	0	2.608690	3.964380	-0.934148
17	1	0	0.271318	2.984429	-0.651861
18	1	0	5.135447	-0.095810	-0.524808
19	1	0	4.950976	0.490568	1.133055
20	1	0	3.604247	-1.432243	1.756194
21	1	0	4.909334	-2.091302	0.756569
22	1	0	3.378939	-1.911015	-1.254590
23	1	0	2.668427	-2.955394	-0.010720
24	1	0	1.213325	2.854871	0.829855
25	6	0	-4.107881	-0.714793	-0.721748
26	6	0	-5.184461	0.154931	-0.762326
27	6	0	-5.099928	1.357565	-0.060278
28	6	0	-2.936845	-0.411333	-0.017781
29	6	0	-2.861966	0.794794	0.710315

30	6	0	-3.963323	1.666546	0.666917
31	6	0	-1.869638	-1.468924	-0.081180
32	7	0	-1.746701	1.179475	1.448014
33	1	0	-1.946019	1.848802	2.176736
34	1	0	-4.138851	-1.669283	-1.236871
35	1	0	-6.075699	-0.097596	-1.325250
36	1	0	-5.930142	2.057237	-0.071414
37	1	0	-3.909828	2.598262	1.224156
38	8	0	-2.149003	-2.632439	-0.254181
39	1	0	-0.344105	0.028655	-0.130484
40	7	0	-0.561614	-0.983743	0.020773
41	1	0	-1.131826	0.438972	1.753222

TBD-$\mathbf{TS_{8/9}}$

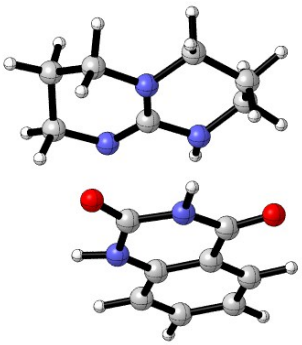
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.648323	-2.280501	0.445428
2	6	0	0.196227	-1.139752	0.315176
3	6	0	-3.936287	1.500219	-0.091464
4	6	0	-2.976724	2.665758	0.069335
5	6	0	-1.820552	2.470364	-0.904056
6	7	0	-3.216343	0.235187	-0.012139
7	6	0	-1.866901	0.183160	-0.281500
8	7	0	-1.172725	1.184744	-0.724244
9	6	0	-4.020436	-0.951362	0.234849
10	6	0	-3.370010	-2.151898	-0.426246
11	6	0	-1.958502	-2.294935	0.104667
12	7	0	-1.225276	-1.034002	-0.049665
13	1	0	-4.472575	1.569990	-1.050948
14	1	0	-4.688349	1.502571	0.706997
15	1	0	-2.589515	2.685707	1.094874
16	1	0	-3.498756	3.609660	-0.116301
17	1	0	-1.067562	3.253208	-0.769495
18	1	0	-4.141934	-1.123763	1.315538
19	1	0	-5.017089	-0.767848	-0.184140

20	1	0	-3.357546	-2.006004	-1.513382
21	1	0	-3.937174	-3.062447	-0.211190
22	1	0	-1.984066	-2.584019	1.164378
23	1	0	-1.404128	-3.073861	-0.421253
24	1	0	-2.192297	2.560185	-1.936940
25	6	0	4.094263	0.518065	0.757640
26	6	0	5.050761	0.408008	-0.246293
27	6	0	4.664621	0.032674	-1.533199
28	6	0	2.752212	0.257411	0.484763
29	6	0	2.371608	-0.094378	-0.811907
30	6	0	3.324564	-0.216980	-1.819004
31	6	0	1.760688	0.344086	1.605182
32	7	0	0.983226	-0.336173	-1.060801
33	1	0	0.833764	-0.957648	-1.855552
34	1	0	4.360633	0.795700	1.772843
35	1	0	6.095336	0.605739	-0.026909
36	1	0	5.407244	-0.065775	-2.319446
37	1	0	3.016804	-0.501198	-2.822134
38	8	0	2.059154	0.834517	2.684376
39	1	0	-0.096114	-0.149362	2.149134
40	7	0	0.503888	-0.110780	1.330145
41	1	0	0.370920	0.521572	-1.145237

TBD-**9**



Standard orientation:

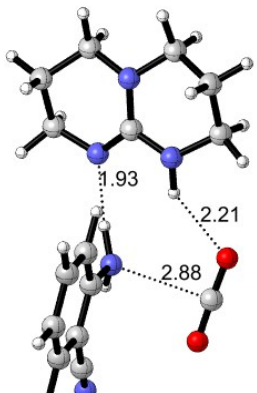
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.843298	-1.624792	2.166389
2	6	0	0.112877	-1.042856	1.687029
3	6	0	-2.876095	1.724168	-0.036198
4	6	0	-1.724214	2.713902	-0.107104
5	6	0	-0.854859	2.388094	-1.311417
6	7	0	-2.424598	0.344196	-0.169391
7	6	0	-1.311325	-0.014699	-0.899014
8	7	0	-0.412577	1.009595	-1.187028
9	6	0	-3.409502	-0.684442	0.165112

10	6	0	-3.330031	-1.844401	-0.816806
11	6	0	-1.876549	-2.296984	-0.917192
12	7	0	-0.977061	-1.208585	-1.254449
13	1	0	-3.617044	1.950881	-0.822183
14	1	0	-3.392545	1.812984	0.927078
15	1	0	-1.105929	2.662006	0.795009
16	1	0	-2.122710	3.730411	-0.185314
17	1	0	0.032918	3.027288	-1.325604
18	1	0	-3.231998	-1.038165	1.189208
19	1	0	-4.401898	-0.219123	0.130548
20	1	0	-3.678826	-1.514956	-1.803702
21	1	0	-3.977311	-2.661617	-0.482058
22	1	0	-1.581052	-2.748634	0.043512
23	1	0	-1.770838	-3.072326	-1.684215
24	1	0	-1.419548	2.561093	-2.243353
25	6	0	3.227069	1.061428	-0.289958
26	6	0	4.095741	0.369864	-1.120535
27	6	0	3.955159	-1.017167	-1.259395
28	6	0	2.226359	0.378066	0.404562
29	6	0	2.094686	-1.008595	0.268426
30	6	0	2.967936	-1.707855	-0.572328
31	6	0	1.258357	1.120362	1.233112
32	7	0	1.105870	-1.675444	0.980270
33	1	0	0.887294	-2.632651	0.731963
34	1	0	3.293427	2.137798	-0.159896
35	1	0	4.876101	0.896312	-1.660074
36	1	0	4.625798	-1.566029	-1.914204
37	1	0	2.859304	-2.782692	-0.688029
38	8	0	1.259707	2.327072	1.394840
39	1	0	-0.416786	0.793602	2.381526
40	7	0	0.310249	0.319336	1.856546
41	1	0	0.263527	0.688595	-1.871440

TBD-**10**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

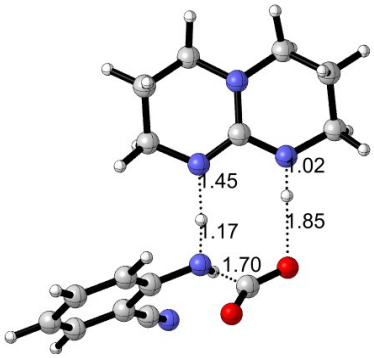


1	6	0	1.985492	-0.589309	0.036303
2	6	0	1.237867	-0.712775	1.221964
3	6	0	1.866011	-1.003871	2.423368
4	6	0	3.253708	-1.175721	2.496450
5	6	0	3.383801	-0.767089	0.117713
6	6	0	4.006943	-1.055414	1.339408
7	1	0	3.734670	-1.398383	3.442905
8	1	0	1.264375	-1.094668	3.323787
9	7	0	1.365017	-0.232565	-1.147497
10	1	0	1.914696	-0.387041	-1.987125
11	1	0	5.084924	-1.183849	1.358414
12	1	0	0.161480	-0.568848	1.175044
13	6	0	4.154147	-0.660265	-1.087790
14	7	0	4.724469	-0.578014	-2.093809
15	1	0	-0.670745	1.229557	-0.458379
16	6	0	-2.180929	-0.079979	-0.344222
17	7	0	-1.496520	-0.940476	-1.024494
18	7	0	-1.547473	1.090065	0.032939
19	6	0	-4.192157	-1.437710	-0.324008
20	6	0	-3.236542	-2.615085	-0.438218
21	6	0	-2.089898	-2.224101	-1.363815
22	6	0	-4.291844	0.871496	0.526698
23	6	0	-3.463182	1.934363	1.231383
24	6	0	-2.286248	2.302731	0.344080
25	1	0	0.384171	-0.542811	-1.235015
26	1	0	-1.300656	-2.983764	-1.330044
27	1	0	-2.447294	-2.193295	-2.403865
28	1	0	-3.763938	-3.496359	-0.817747
29	1	0	-2.846608	-2.855234	0.558031
30	1	0	-4.986733	-1.641501	0.402347
31	1	0	-4.673807	-1.237799	-1.296276
32	1	0	-5.078577	0.492800	1.188601
33	1	0	-4.788934	1.305736	-0.358208
34	1	0	-3.093678	1.540832	2.184581
35	1	0	-4.082592	2.813189	1.435407
36	1	0	-1.604180	2.989371	0.851978
37	1	0	-2.648618	2.804309	-0.568133
38	6	0	1.975046	2.535397	-0.634769
39	8	0	3.097658	2.297916	-0.804777

40	8	0	0.858046	2.820704	-0.454697
41	7	0	-3.465046	-0.264326	0.138893

TBD-**TS**$_{10/11}$

Standard orientation:

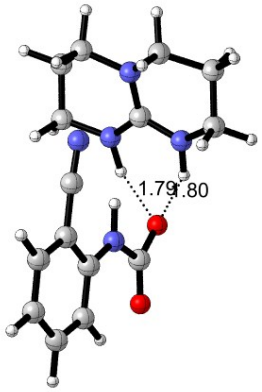


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.352036	-0.106894	-0.135864
2	6	0	2.448750	0.480710	-1.398125
3	6	0	3.547586	1.270605	-1.715780
4	6	0	4.567935	1.484682	-0.785799
5	6	0	3.377508	0.109959	0.798615
6	6	0	4.483299	0.905099	0.472150
7	1	0	5.425629	2.097112	-1.043739
8	1	0	3.614929	1.716247	-2.703699
9	7	0	1.216313	-0.899357	0.169978
10	1	0	1.244341	-1.269391	1.123549
11	1	0	5.261486	1.056632	1.213142
12	1	0	1.666321	0.290516	-2.125642
13	6	0	3.270126	-0.479513	2.105448
14	7	0	3.139300	-0.961001	3.150961
15	1	0	-1.548816	-1.779359	-0.152871
16	6	0	-2.166968	0.141222	0.039797
17	7	0	-0.931401	0.581067	-0.016633
18	7	0	-2.382126	-1.192561	-0.061189
19	6	0	-3.064887	2.377158	0.422237
20	6	0	-1.823569	2.870504	-0.303267
21	6	0	-0.643334	2.003064	0.111964
22	6	0	-4.587319	0.419362	0.430213
23	6	0	-4.780224	-0.918041	-0.266746
24	6	0	-3.656871	-1.850506	0.153361
25	1	0	0.228214	-0.276163	0.077677
26	1	0	0.233293	2.231814	-0.503951
27	1	0	-0.365617	2.233020	1.152133
28	1	0	-1.636480	3.921461	-0.061696
29	1	0	-1.983641	2.790624	-1.384609

30	1	0	-3.958240	2.908071	0.077020
31	1	0	-2.972723	2.550908	1.506479
32	1	0	-5.321763	1.149207	0.073846
33	1	0	-4.732413	0.308517	1.517192
34	1	0	-4.755291	-0.771253	-1.352049
35	1	0	-5.752018	-1.341845	0.003331
36	1	0	-3.662839	-2.769601	-0.437830
37	1	0	-3.778160	-2.132864	1.209718
38	6	0	0.910850	-2.250653	-0.817795
39	8	0	1.655792	-2.302477	-1.759217
40	8	0	-0.038493	-2.832518	-0.312006
41	7	0	-3.264101	0.961248	0.145359

TBD-**11**

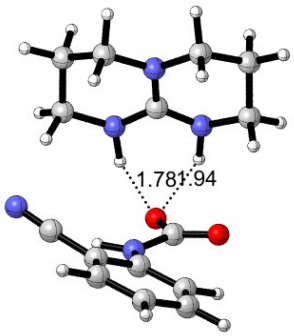
Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.524538	0.039875	-0.001420
2	6	0	-3.868226	0.466936	0.000263
3	6	0	-4.889356	-0.469832	0.001682
4	6	0	-4.641657	-1.850542	0.001521
5	6	0	-2.282585	-1.360562	-0.001468
6	6	0	-3.331017	-2.291639	-0.000061
7	1	0	-5.461554	-2.560599	0.002642
8	1	0	-5.916087	-0.113847	0.002941
9	7	0	-1.444918	0.883663	-0.003016
10	1	0	-0.537699	0.435455	-0.004443
11	1	0	-3.094352	-3.351497	-0.000205
12	1	0	-4.068369	1.530536	0.000401
13	6	0	-0.918674	-1.790535	-0.002882
14	7	0	0.218358	-2.030947	-0.003983
15	1	0	0.981618	1.810339	1.017863
16	6	0	2.088212	0.487290	0.000530
17	7	0	1.674007	1.044828	-1.143876
18	7	0	1.671477	1.046030	1.143383
19	6	0	3.205060	-1.288028	-1.238168

20	6	0	3.189695	-0.341750	-2.430181
21	6	0	1.877067	0.426121	-2.444877
22	6	0	3.200866	-1.287328	1.243510
23	6	0	3.183882	-0.339846	2.434550
24	6	0	1.872013	0.429389	2.445739
25	1	0	0.984000	1.809334	-1.020801
26	1	0	1.890725	1.219936	-3.195253
27	1	0	1.040263	-0.247657	-2.673444
28	1	0	3.303316	-0.914735	-3.354651
29	1	0	4.027462	0.360473	-2.357344
30	1	0	4.189678	-1.753077	-1.129193
31	1	0	2.456583	-2.083422	-1.353790
32	1	0	4.185080	-1.753888	1.137430
33	1	0	2.450980	-2.081598	1.357962
34	1	0	4.022567	0.361379	2.362731
35	1	0	3.294930	-0.911956	3.359872
36	1	0	1.885304	1.224462	3.194799
37	1	0	1.034128	-0.243060	2.674217
38	6	0	-1.379602	2.331341	-0.001915
39	8	0	-2.423818	2.966736	-0.000288
40	8	0	-0.168329	2.735550	-0.002765
41	7	0	2.935614	-0.560745	0.002026

TBD-$\mathbf{TS_{11/12}}$



Standard orientation:

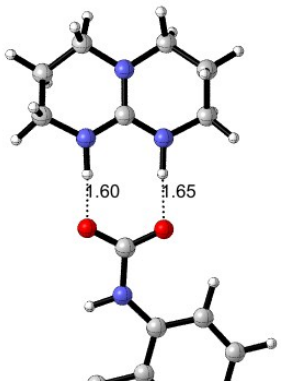
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.444960	-0.214064	0.370523
2	6	0	3.071347	-1.395242	-0.069230
3	6	0	4.057785	-1.338993	-1.042177
4	6	0	4.465561	-0.126621	-1.613226
5	6	0	2.838357	1.002876	-0.236459
6	6	0	3.849431	1.044625	-1.207294
7	1	0	5.248992	-0.102713	-2.363452
8	1	0	4.532651	-2.264574	-1.356368
9	7	0	1.494550	-0.194227	1.369403

10	1	0	1.294099	0.696015	1.808424
11	1	0	4.126516	2.002846	-1.636590
12	1	0	2.762587	-2.335375	0.368808
13	6	0	2.131526	2.199371	0.115161
14	7	0	1.503606	3.131217	0.405617
15	1	0	-1.391832	0.380939	2.016485
16	6	0	-2.200496	-0.108673	0.268141
17	7	0	-2.139291	-1.409930	0.578620
18	7	0	-1.930849	0.781623	1.228309
19	6	0	-2.656292	-0.664001	-2.071582
20	6	0	-3.032907	-2.051278	-1.573417
21	6	0	-2.098714	-2.449625	-0.443099
22	6	0	-2.452693	1.702278	-1.330263
23	6	0	-2.810527	2.586070	-0.145236
24	6	0	-1.914113	2.227149	1.028483
25	1	0	-1.659525	-1.611379	1.465112
26	1	0	-2.417417	-3.382273	0.026470
27	1	0	-1.065310	-2.584541	-0.786033
28	1	0	-2.960752	-2.765130	-2.398664
29	1	0	-4.068356	-2.045579	-1.215500
30	1	0	-3.402324	-0.287349	-2.778345
31	1	0	-1.686180	-0.691256	-2.589499
32	1	0	-3.129930	1.882545	-2.170340
33	1	0	-1.426417	1.906565	-1.670166
34	1	0	-3.863094	2.431644	0.117417
35	1	0	-2.672597	3.637662	-0.410229
36	1	0	-2.269971	2.696086	1.949676
37	1	0	-0.887815	2.568331	0.846194
38	6	0	0.575260	-1.231634	1.725428
39	8	0	0.635485	-2.311943	1.125121
40	8	0	-0.269151	-0.867012	2.600677
41	7	0	-2.585860	0.292141	-0.965421

TBD-**12**

Standard orientation:

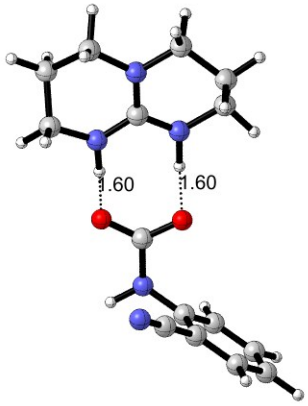
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	8	0	0.555566	-0.708663	-0.074658
2	6	0	0.941206	0.487108	-0.068491
3	8	0	0.222369	1.520631	-0.076753
4	7	0	2.323497	0.757926	-0.048651
5	1	0	-1.356701	1.297177	-0.162936
6	6	0	3.399774	-0.106748	-0.024511
7	6	0	3.288651	-1.508959	-0.060725
8	6	0	4.703777	0.444012	0.036892
9	6	0	4.428542	-2.301242	-0.035829
10	1	0	2.302378	-1.947942	-0.108922
11	6	0	5.841369	-0.371832	0.060799
12	6	0	5.712036	-1.750757	0.024919
13	1	0	4.309111	-3.381030	-0.065845
14	1	0	6.818688	0.098786	0.109418
15	1	0	6.590835	-2.386428	0.042895
16	6	0	4.862035	1.869562	0.077068
17	7	0	4.954161	3.024960	0.109126
18	1	0	2.523050	1.751820	-0.034284
19	1	0	-1.077691	-0.888699	0.018387
20	6	0	-4.893323	-1.507931	0.102334
21	6	0	-3.930039	-2.591222	-0.359357
22	6	0	-2.598323	-2.399509	0.352256
23	7	0	-4.280116	-0.183233	0.031612
24	6	0	-2.935512	-0.012313	-0.024217
25	7	0	-2.115337	-1.056892	0.092932
26	6	0	-5.204764	0.949080	0.037384
27	6	0	-4.503680	2.238208	0.438016
28	6	0	-3.231138	2.380840	-0.384587
29	7	0	-2.412591	1.197893	-0.199721
30	1	0	-5.222620	-1.698361	1.134051
31	1	0	-5.787335	-1.491065	-0.531916
32	1	0	-3.776142	-2.517601	-1.441580
33	1	0	-4.354825	-3.574800	-0.139625
34	1	0	-1.842997	-3.097367	-0.015755
35	1	0	-5.658330	1.049718	-0.958910
36	1	0	-6.008773	0.712339	0.744260
37	1	0	-4.245407	2.208466	1.502237
38	1	0	-5.175785	3.084849	0.271907
39	1	0	-3.477562	2.518239	-1.446955

40	1	0	-2.639084	3.241512	-0.065935
41	1	0	-2.715263	-2.569708	1.432009

TBD-**TS**$_{12/13}$

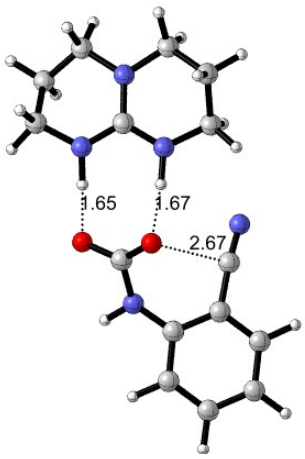


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.866505	0.337134	-0.750984
2	6	0	1.071124	-0.894875	-0.910784
3	8	0	0.214475	-1.806013	-1.048825
4	7	0	2.417369	-1.309643	-0.965017
5	1	0	-1.259625	-1.385635	-0.583794
6	6	0	3.443128	-0.447483	-0.501213
7	6	0	4.265779	0.210296	-1.411510
8	6	0	3.651418	-0.230624	0.871625
9	6	0	5.280636	1.056854	-0.970712
10	1	0	4.086903	0.045760	-2.469238
11	6	0	4.671683	0.615252	1.318599
12	6	0	5.486909	1.258262	0.393814
13	1	0	5.913839	1.561175	-1.694998
14	1	0	4.813252	0.763098	2.384753
15	1	0	6.279319	1.915952	0.737447
16	6	0	2.794286	-0.883636	1.826992
17	7	0	2.118096	-1.406783	2.607953
18	1	0	2.534495	-2.301449	-0.792981
19	1	0	-0.678789	0.751675	-0.650913
20	6	0	-4.215972	1.892388	0.397930
21	6	0	-2.990673	2.771356	0.600251
22	6	0	-1.990821	2.480921	-0.510464
23	7	0	-3.842360	0.497607	0.174144
24	6	0	-2.585406	0.138938	-0.194250
25	7	0	-1.684342	1.064286	-0.517561
26	6	0	-4.896499	-0.487378	0.407542
27	6	0	-4.552481	-1.833943	-0.212699
28	6	0	-3.128473	-2.203584	0.177996
29	7	0	-2.236543	-1.143803	-0.247293

30	1	0	-4.809958	2.248387	-0.456266
31	1	0	-4.861787	1.921721	1.283727
32	1	0	-2.528268	2.551780	1.568916
33	1	0	-3.291790	3.822906	0.594326
34	1	0	-1.051404	3.016695	-0.356357
35	1	0	-5.054315	-0.592775	1.490701
36	1	0	-5.822818	-0.088210	-0.023169
37	1	0	-4.623387	-1.772833	-1.304227
38	1	0	-5.265499	-2.586487	0.136071
39	1	0	-3.058084	-2.359326	1.263945
40	1	0	-2.802218	-3.123233	-0.312500
41	1	0	-2.401076	2.793719	-1.481253

TBD-**13**



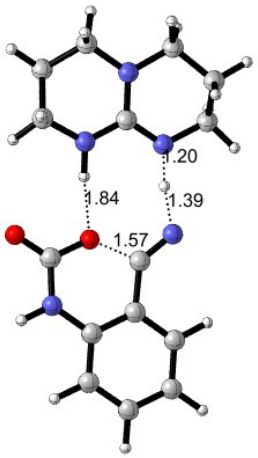
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.878010	-0.336513	-0.904917
2	6	0	-1.048200	-1.363170	-0.207546
3	8	0	-0.216501	-2.268283	0.054228
4	7	0	-2.328506	-1.543486	0.377555
5	1	0	1.288556	-1.670146	-0.285957
6	6	0	-3.427868	-0.721061	0.168915
7	6	0	-4.680459	-1.287081	-0.109152
8	6	0	-3.350596	0.683161	0.284275
9	6	0	-5.805363	-0.495269	-0.295092
10	1	0	-4.752310	-2.367939	-0.198283
11	6	0	-4.486465	1.475188	0.068127
12	6	0	-5.712522	0.896013	-0.226018
13	1	0	-6.759080	-0.967536	-0.513128
14	1	0	-4.391094	2.553208	0.157243
15	1	0	-6.586493	1.518349	-0.387961
16	6	0	-2.153884	1.349495	0.723618
17	7	0	-1.254472	1.956241	1.131166
18	1	0	-2.509733	-2.494976	0.669633
19	1	0	0.561166	0.431818	-0.557334

20	6	0	4.092525	1.862848	0.014323
21	6	0	3.000000	2.688192	-0.649503
22	6	0	1.649758	2.256375	-0.095506
23	7	0	3.772788	0.435794	0.003696
24	6	0	2.514314	-0.021243	-0.213936
25	7	0	1.497158	0.829063	-0.313491
26	6	0	4.887737	-0.462069	0.297365
27	6	0	4.399261	-1.836418	0.730025
28	6	0	3.345212	-2.313359	-0.259827
29	7	0	2.283353	-1.329172	-0.341412
30	1	0	4.238716	2.186360	1.054970
31	1	0	5.048351	1.989992	-0.508463
32	1	0	3.016617	2.528772	-1.733446
33	1	0	3.181587	3.749468	-0.457227
34	1	0	0.821130	2.754862	-0.600407
35	1	0	5.528779	-0.542160	-0.592334
36	1	0	5.483200	0.003322	1.092043
37	1	0	3.955518	-1.778279	1.730026
38	1	0	5.245717	-2.528126	0.769270
39	1	0	3.797978	-2.475237	-1.248053
40	1	0	2.890421	-3.253988	0.058874
41	1	0	1.564114	2.491919	0.973050

TBD-**TS$_{13/14}$**

Standard orientation:



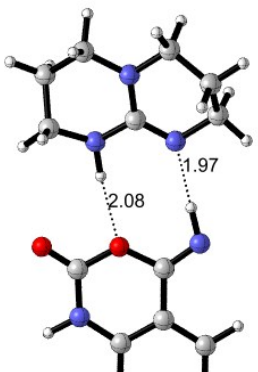
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.606351	-1.376454	-0.272302
2	6	0	4.578729	-1.407452	0.265695
3	6	0	3.666371	-2.590450	0.556709
4	6	0	2.508167	-2.561767	-0.432118
5	7	0	3.814747	-0.172813	0.103316
6	6	0	2.465089	-0.187423	-0.086245
7	7	0	1.801335	-1.300737	-0.326198
8	6	0	4.586130	1.062251	0.219742
9	6	0	3.811679	2.265905	-0.298433

10	6	0	2.414814	2.242178	0.305152
11	7	0	1.795164	0.976977	-0.033649
12	1	0	5.164738	-1.589809	-0.646911
13	1	0	5.289792	-1.253080	1.087279
14	1	0	3.270030	-2.516742	1.575590
15	1	0	4.238159	-3.520050	0.478314
16	1	0	1.783039	-3.354989	-0.228823
17	1	0	4.863602	1.214183	1.273701
18	1	0	5.515896	0.926498	-0.346999
19	1	0	3.734165	2.222452	-1.390412
20	1	0	4.343703	3.182754	-0.028209
21	1	0	2.471822	2.369544	1.396134
22	1	0	1.773323	3.032619	-0.089216
23	1	0	2.885476	-2.710653	-1.454943
24	8	0	-0.997189	0.692972	-0.534469
25	6	0	-1.555918	1.834032	-0.158470
26	8	0	-0.929608	2.878767	-0.103114
27	7	0	-2.893597	1.758467	0.151134
28	6	0	-3.650361	0.586351	0.114748
29	6	0	-5.037019	0.641454	0.286232
30	6	0	-3.014824	-0.648175	-0.069556
31	6	0	-5.783876	-0.529879	0.272138
32	1	0	-5.521897	1.603892	0.429923
33	6	0	-3.780083	-1.816428	-0.074676
34	6	0	-5.158999	-1.765716	0.088487
35	1	0	-6.860727	-0.476461	0.403785
36	1	0	-3.256935	-2.758780	-0.207368
37	1	0	-5.744766	-2.679260	0.076450
38	6	0	-1.548782	-0.743799	-0.205962
39	7	0	-0.748814	-1.655951	-0.150756
40	1	0	-3.331343	2.633871	0.404115
41	1	0	0.801398	0.948464	-0.267025

TBD-**14**

Standard orientation:

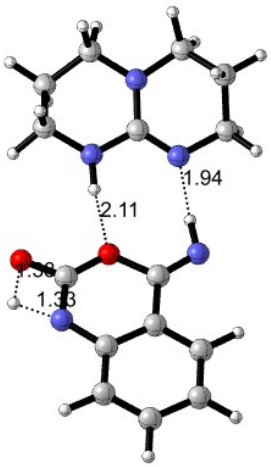
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z



1	1	0	-0.035922	-1.586620	-0.449711
2	8	0	-1.017733	0.525446	-0.210591
3	6	0	-1.570707	1.746689	-0.028534
4	8	0	-0.868372	2.729041	-0.018024
5	7	0	-2.928008	1.772062	0.131724
6	6	0	-3.750386	0.642988	0.121021
7	6	0	-5.132302	0.760173	0.281608
8	6	0	-3.161707	-0.611207	-0.051943
9	6	0	-5.917951	-0.385619	0.268684
10	1	0	-5.582059	1.740466	0.415157
11	6	0	-3.962983	-1.754551	-0.062199
12	6	0	-5.338042	-1.646390	0.097402
13	1	0	-6.992829	-0.293690	0.393338
14	1	0	-3.475864	-2.715101	-0.197831
15	1	0	-5.959067	-2.535961	0.088962
16	6	0	-1.701755	-0.709856	-0.216295
17	7	0	-1.054858	-1.771729	-0.357457
18	1	0	-3.326454	2.692446	0.264448
19	6	0	4.647412	-1.421961	0.407044
20	6	0	3.666908	-2.548463	0.696093
21	6	0	2.597478	-2.550336	-0.391265
22	7	0	3.949048	-0.188308	0.065303
23	6	0	2.609414	-0.208745	-0.264308
24	7	0	1.904723	-1.278132	-0.461706
25	6	0	4.714069	1.027049	0.315975
26	6	0	4.031579	2.270931	-0.233729
27	6	0	2.558778	2.219583	0.141616
28	7	0	2.008053	1.016395	-0.446700
29	1	0	5.321710	-1.700831	-0.416667
30	1	0	5.274886	-1.221549	1.286216
31	1	0	3.186732	-2.382977	1.667854
32	1	0	4.203214	-3.502245	0.740073
33	1	0	1.856259	-3.334409	-0.201086
34	1	0	4.866203	1.137370	1.402539
35	1	0	5.707279	0.900752	-0.135468
36	1	0	4.117823	2.301094	-1.325202
37	1	0	4.517580	3.161524	0.177113
38	1	0	2.447962	2.236285	1.239178
39	1	0	2.006049	3.071906	-0.259469

40	1	0	3.065265	-2.786982	-1.361613
41	1	0	0.998528	0.948889	-0.504078

TBD-$\mathbf{TS}_{14/15}$



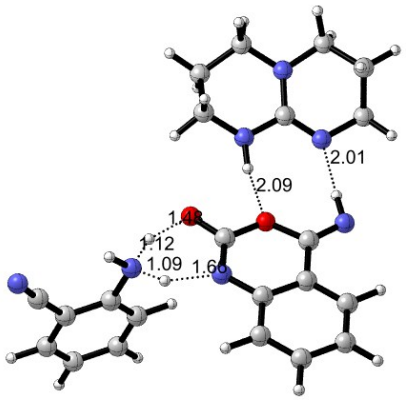
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.001076	-1.532389	-0.444085
2	8	0	-1.008059	0.579201	-0.202992
3	6	0	-1.700118	1.682319	-0.031164
4	8	0	-1.186906	2.847230	0.006561
5	7	0	-3.002126	1.776553	0.127085
6	6	0	-3.796806	0.634496	0.120220
7	6	0	-5.182497	0.698360	0.275894
8	6	0	-3.158642	-0.606864	-0.049745
9	6	0	-5.924945	-0.475494	0.261524
10	1	0	-5.654399	1.667034	0.405904
11	6	0	-3.920472	-1.777818	-0.061251
12	6	0	-5.299290	-1.715441	0.093547
13	1	0	-7.003229	-0.425544	0.382330
14	1	0	-3.404654	-2.723867	-0.193791
15	1	0	-5.888312	-2.626706	0.083887
16	6	0	-1.692909	-0.691012	-0.212693
17	7	0	-1.016495	-1.729510	-0.353583
18	1	0	-2.499415	3.011189	0.170454
19	6	0	4.667020	-1.443363	0.391604
20	6	0	3.671620	-2.555198	0.686406
21	6	0	2.593599	-2.540502	-0.392341
22	7	0	3.984313	-0.197272	0.061182
23	6	0	2.644988	-0.198785	-0.262876
24	7	0	1.922751	-1.255724	-0.459420
25	6	0	4.765471	1.007022	0.316753
26	6	0	4.099024	2.261705	-0.227777
27	6	0	2.626134	2.230277	0.149849
28	7	0	2.058028	1.035914	-0.441542
29	1	0	5.328588	-1.728905	-0.439784

30	1	0	5.305521	-1.255539	1.265308
31	1	0	3.202024	-2.384385	1.662375
32	1	0	4.193613	-3.516982	0.724573
33	1	0	1.839952	-3.310605	-0.194967
34	1	0	4.919822	1.110489	1.403465
35	1	0	5.756118	0.870068	-0.136570
36	1	0	4.183692	2.294561	-1.319188
37	1	0	4.597134	3.144322	0.185371
38	1	0	2.517218	2.246447	1.247343
39	1	0	2.089713	3.093652	-0.250820
40	1	0	3.048168	-2.785726	-1.366448
41	1	0	1.048731	0.973513	-0.497678

TBD-$\mathbf{TS_{14/15}}$'

Standard orientation:



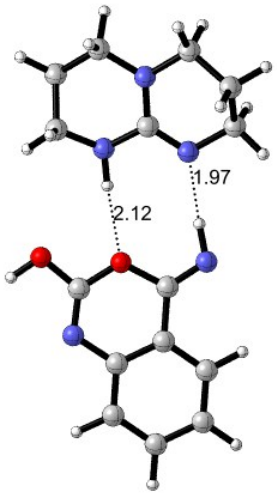
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.247465	-1.181193	-0.194184
2	6	0	6.239090	0.339851	-0.199853
3	6	0	5.331912	0.822938	0.926918
4	7	0	4.897599	-1.717453	-0.060296
5	6	0	3.856940	-0.901407	0.340306
6	7	0	3.984721	0.306337	0.786655
7	6	0	4.728754	-3.059893	-0.599595
8	6	0	3.360832	-3.647031	-0.284558
9	6	0	2.305862	-2.585680	-0.555300
10	7	0	2.595346	-1.459060	0.306928
11	1	0	6.875120	-1.559530	0.626959
12	1	0	6.671997	-1.567527	-1.130940
13	1	0	5.844248	0.706056	-1.154982
14	1	0	7.261686	0.715487	-0.088256
15	1	0	5.280362	1.917311	0.936449
16	1	0	4.875981	-3.029283	-1.692297
17	1	0	5.525244	-3.694439	-0.187387
18	1	0	3.306920	-3.938379	0.770058
19	1	0	3.199071	-4.538756	-0.898797

20	1	0	2.314614	-2.308966	-1.623706
21	1	0	1.300914	-2.939683	-0.314974
22	1	0	5.760573	0.517946	1.896325
23	1	0	1.865566	-0.759655	0.396650
24	1	0	-1.930007	-1.190563	-0.787987
25	1	0	-2.771064	0.136714	-0.973636
26	1	0	2.713602	1.865975	0.716271
27	8	0	0.675358	0.926904	0.082850
28	6	0	-0.525538	0.430426	-0.302514
29	8	0	-0.549397	-0.833038	-0.375326
30	7	0	-1.564735	1.202967	-0.559610
31	6	0	-1.423363	2.583446	-0.441320
32	6	0	-2.519791	3.414382	-0.714302
33	6	0	-0.209145	3.170087	-0.055919
34	6	0	-2.397672	4.791989	-0.604647
35	1	0	-3.459128	2.958030	-1.014960
36	6	0	-0.092931	4.558174	0.053056
37	6	0	-1.182733	5.372594	-0.220064
38	1	0	-3.254804	5.423282	-0.822489
39	1	0	0.866404	4.967853	0.354881
40	1	0	-1.093619	6.451174	-0.136940
41	6	0	0.939204	2.299787	0.229642
42	7	0	2.084093	2.676985	0.580985
43	7	0	-3.000431	-0.932421	-0.984610
44	6	0	-3.859412	-1.304885	0.107224
45	6	0	-5.048435	-2.009314	-0.115285
46	6	0	-5.866423	-2.360605	0.965083
47	6	0	-5.493308	-2.004130	2.254393
48	6	0	-4.307260	-1.299960	2.467200
49	6	0	-3.486298	-0.949111	1.399112
50	1	0	-6.784327	-2.907698	0.776996
51	6	0	-5.406922	-2.360284	-1.462322
52	1	0	-2.559091	-0.405006	1.554740
53	1	0	-4.014676	-1.021717	3.474669
54	1	0	-6.125113	-2.275239	3.093553
55	7	0	-5.638659	-2.611937	-2.568774
56	1	0	-3.328667	-1.253346	-1.897767

TBD-**15**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.034841	-1.563719	-0.446541
2	8	0	-1.057596	0.548723	-0.201138
3	6	0	-1.750949	1.677909	-0.036956
4	8	0	-0.902304	2.711173	-0.055235
5	7	0	-3.004526	1.825663	0.117315
6	6	0	-3.768949	0.649433	0.115017
7	6	0	-5.154882	0.743897	0.274922
8	6	0	-3.176697	-0.612236	-0.042175
9	6	0	-5.931678	-0.406821	0.277388
10	1	0	-5.595585	1.728527	0.395527
11	6	0	-3.963973	-1.766640	-0.038497
12	6	0	-5.339138	-1.665594	0.121049
13	1	0	-7.007885	-0.327029	0.401692
14	1	0	-3.472001	-2.726347	-0.163178
15	1	0	-5.952594	-2.561056	0.123723
16	6	0	-1.718771	-0.709504	-0.209344
17	7	0	-1.049534	-1.757016	-0.350721
18	1	0	-1.437126	3.514424	0.060463
19	6	0	4.661127	-1.434488	0.384689
20	6	0	3.678718	-2.559875	0.672416
21	6	0	2.602706	-2.554400	-0.408432
22	7	0	3.963585	-0.194394	0.062112
23	6	0	2.624713	-0.213317	-0.267712
24	7	0	1.918673	-1.277040	-0.475146
25	6	0	4.723415	1.017835	0.339374
26	6	0	4.041792	2.267691	-0.197015
27	6	0	2.566379	2.209380	0.167736
28	7	0	2.019251	1.015316	-0.441637
29	1	0	5.326234	-1.707296	-0.448169
30	1	0	5.297058	-1.244751	1.259874
31	1	0	3.205111	-2.398557	1.648079
32	1	0	4.212439	-3.515313	0.708054
33	1	0	1.856576	-3.332402	-0.213971

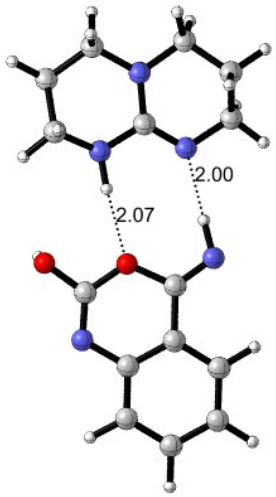


34	1	0	4.866996	1.111804	1.428648
35	1	0	5.720147	0.902407	-0.106623
36	1	0	4.134459	2.312918	-1.287375
37	1	0	4.522852	3.153670	0.229205
38	1	0	2.448498	2.213505	1.264912
39	1	0	2.022566	3.070099	-0.229255
40	1	0	3.061460	-2.792893	-1.382208
41	1	0	1.009818	0.935523	-0.490085

TBD-$\mathbf{TS_{15/16}}$

Standard orientation:

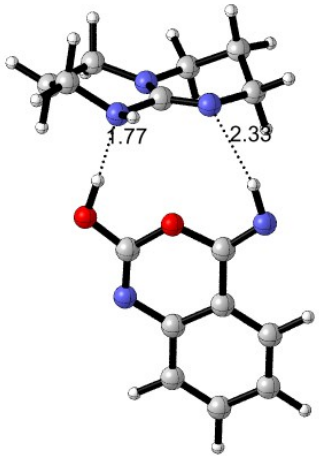
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.050317	-1.607459	-0.263843
2	8	0	-1.076033	0.508074	-0.229947
3	6	0	-1.768789	1.664761	-0.253915
4	8	0	-0.914283	2.709047	-0.354017
5	7	0	-3.020566	1.815944	-0.149532
6	6	0	-3.780725	0.643474	0.011519
7	6	0	-5.166414	0.761667	0.153979
8	6	0	-3.189028	-0.627071	0.029035
9	6	0	-5.944606	-0.377205	0.312106
10	1	0	-5.603739	1.755068	0.137425
11	6	0	-3.976416	-1.769799	0.185956
12	6	0	-5.351795	-1.645332	0.328051
13	1	0	-7.020827	-0.281387	0.423649
14	1	0	-3.485380	-2.738172	0.193695
15	1	0	-5.966352	-2.531910	0.451035
16	6	0	-1.730868	-0.740226	-0.119834
17	7	0	-1.061950	-1.799335	-0.148408
18	1	0	-0.736247	2.916722	-1.284806
19	6	0	4.728026	-1.404144	0.130085
20	6	0	3.804024	-2.584220	0.390457
21	6	0	2.626850	-2.500494	-0.575518
22	7	0	3.973749	-0.159522	0.023245
23	6	0	2.610219	-0.188990	-0.179711



24	7	0	1.911651	-1.245682	-0.438628
25	6	0	4.729456	1.038663	0.367756
26	6	0	3.962031	2.319713	0.074003
27	6	0	2.533307	2.151728	0.566894
28	7	0	1.960651	1.032060	-0.153444
29	1	0	5.305252	-1.563389	-0.792969
30	1	0	5.450114	-1.290513	0.949647
31	1	0	3.426023	-2.538627	1.418764
32	1	0	4.358247	-3.521171	0.273162
33	1	0	1.920632	-3.318087	-0.394982
34	1	0	4.991067	1.001072	1.438024
35	1	0	5.672897	1.018355	-0.193841
36	1	0	3.943410	2.513421	-1.003844
37	1	0	4.459362	3.160025	0.568252
38	1	0	2.527304	1.996840	1.659264
39	1	0	1.928059	3.036608	0.353829
40	1	0	2.992710	-2.620611	-1.608431
41	1	0	0.953945	0.916854	-0.110132

TBD-**16**

Standard orientation:



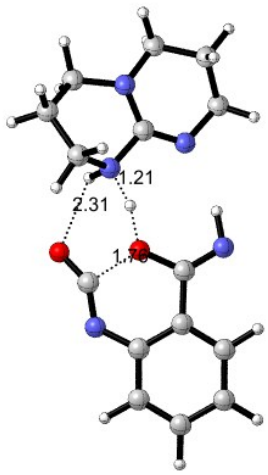
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.336038	1.838591	-1.606979
2	8	0	-0.711842	-0.276390	-0.772118
3	6	0	-0.991494	-1.469769	-0.188403
4	8	0	0.064036	-2.260420	-0.238209
5	7	0	-2.095745	-1.819926	0.339530
6	6	0	-3.118386	-0.867555	0.319092
7	6	0	-4.362384	-1.206908	0.868221
8	6	0	-2.943987	0.417298	-0.222210
9	6	0	-5.397064	-0.283522	0.873190
10	1	0	-4.484285	-2.202038	1.284167
11	6	0	-3.990184	1.344756	-0.213882
12	6	0	-5.216460	0.997096	0.332446
13	1	0	-6.357380	-0.557743	1.301213

14	1	0	-3.814023	2.326658	-0.642813
15	1	0	-6.032509	1.712973	0.340630
16	6	0	-1.639320	0.763255	-0.793997
17	7	0	-1.310848	1.877050	-1.288696
18	1	0	0.829943	-1.743228	-0.630446
19	6	0	3.020235	1.376612	1.645854
20	6	0	3.063543	2.642685	0.801840
21	6	0	1.894784	2.619128	-0.176305
22	7	0	2.900906	0.188033	0.799696
23	6	0	2.356688	0.335922	-0.456788
24	7	0	1.863531	1.400944	-0.971306
25	6	0	3.763163	-0.931552	1.173758
26	6	0	3.462996	-2.189434	0.373874
27	6	0	3.343098	-1.824791	-1.097774
28	7	0	2.246868	-0.857941	-1.214905
29	1	0	2.176563	1.410788	2.348071
30	1	0	3.937338	1.275612	2.236922
31	1	0	4.006934	2.677188	0.242823
32	1	0	3.021478	3.524752	1.448429
33	1	0	1.948143	3.468987	-0.864159
34	1	0	4.817674	-0.641106	1.030429
35	1	0	3.619797	-1.119735	2.243449
36	1	0	2.523553	-2.639397	0.713326
37	1	0	4.264037	-2.918351	0.528842
38	1	0	4.291800	-1.410942	-1.472282
39	1	0	3.087539	-2.698876	-1.702761
40	1	0	0.945448	2.718740	0.371533
41	1	0	2.032076	-0.584831	-2.171511

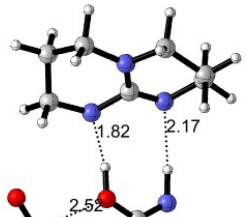
TBD-$\mathbf{TS_{16/18}}$'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.827823	0.861120	-0.160743
2	6	0	-4.298884	2.261107	0.128712
3	6	0	-3.016346	2.504154	-0.666012



4	7	0	-3.773070	-0.112204	0.106245
5	6	0	-2.491746	0.275435	-0.211556
6	7	0	-2.048116	1.420033	-0.530207
7	6	0	-4.100685	-1.530516	-0.023982
8	6	0	-3.172915	-2.395895	0.847385
9	6	0	-1.816226	-1.709746	1.044923
10	7	0	-1.518898	-0.796508	-0.088468
11	1	0	-5.159426	0.783465	-1.208625
12	1	0	-5.681407	0.618275	0.480202
13	1	0	-4.090264	2.348886	1.201255
14	1	0	-5.058301	3.006881	-0.125151
15	1	0	-2.528072	3.426786	-0.339546
16	1	0	-5.142808	-1.652555	0.282015
17	1	0	-4.040633	-1.839539	-1.079374
18	1	0	-3.040704	-3.371646	0.370524
19	1	0	-3.626328	-2.569951	1.827092
20	1	0	-1.809334	-1.086609	1.942230
21	1	0	-0.989441	-2.418941	1.100471
22	1	0	-3.238811	2.628500	-1.733719
23	1	0	-0.393696	-0.374480	0.028047
24	1	0	-1.430777	-1.343182	-0.954137
25	1	0	0.072011	1.980691	0.258402
26	8	0	0.890405	-0.277631	0.141678
27	6	0	1.550288	-1.759505	-0.537017
28	8	0	0.586129	-2.446190	-0.758155
29	7	0	2.803639	-1.710042	-0.589844
30	6	0	3.579589	-0.612986	-0.217705
31	6	0	4.971946	-0.785616	-0.253498
32	6	0	3.064222	0.643043	0.153280
33	6	0	5.826281	0.257248	0.072020
34	1	0	5.353662	-1.757958	-0.548904
35	6	0	3.936268	1.690293	0.467489
36	6	0	5.311071	1.506114	0.434759
37	1	0	6.900948	0.099538	0.039895
38	1	0	3.499536	2.647133	0.737154
39	1	0	5.978118	2.324911	0.686629
40	6	0	1.604014	0.875821	0.195371
41	7	0	1.093462	2.035854	0.291817



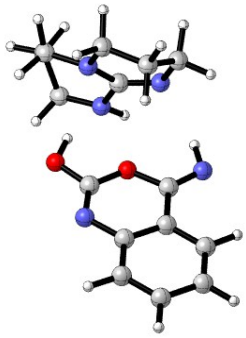
TBD-**18'**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.415316	-1.581370	-0.285305
2	6	0	-3.420930	-2.438257	-1.054144
3	6	0	-2.089966	-2.420344	-0.311640
4	7	0	-3.831958	-0.291589	0.071928
5	6	0	-2.475265	-0.110595	0.051381
6	7	0	-1.605519	-1.062778	-0.141652
7	6	0	-4.796760	0.779362	0.303565
8	6	0	-4.152878	2.014477	0.916876
9	6	0	-2.865547	2.316634	0.165816
10	7	0	-2.008685	1.154342	0.286051
11	1	0	-4.747111	-2.098243	0.627050
12	1	0	-5.307498	-1.384745	-0.893255
13	1	0	-3.276241	-2.025885	-2.059459
14	1	0	-3.811485	-3.455559	-1.155173
15	1	0	-1.330519	-2.985394	-0.861786
16	1	0	-5.276278	1.039899	-0.652924
17	1	0	-5.581088	0.386916	0.963375
18	1	0	-3.916004	1.834479	1.970866
19	1	0	-4.852275	2.853783	0.858665
20	1	0	-3.084894	2.557676	-0.886446
21	1	0	-2.336939	3.167632	0.601050
22	1	0	-2.209969	-2.912880	0.666965
23	1	0	-0.108059	-0.645765	-0.318317
24	1	0	-1.024141	1.289185	0.081297
25	1	0	0.419119	-2.068412	1.183039
26	8	0	0.863737	-0.284974	-0.425888
27	6	0	1.546141	2.155339	-0.445823
28	8	0	0.475559	2.646339	-0.497984
29	7	0	2.690427	1.808541	-0.414076
30	6	0	3.562084	0.739890	-0.196288
31	6	0	4.923338	1.021037	-0.350375
32	6	0	3.142719	-0.543132	0.200156
33	6	0	5.877479	0.041084	-0.113485

34	1	0	5.208611	2.024081	-0.650598
35	6	0	4.124598	-1.507059	0.452714
36	6	0	5.477076	-1.230426	0.295958
37	1	0	6.930558	0.272906	-0.242573
38	1	0	3.786588	-2.485566	0.777676
39	1	0	6.214931	-2.002805	0.489937
40	6	0	1.713077	-0.952239	0.366650
41	7	0	1.425625	-1.888319	1.185642

TBD-$\mathbf{TS}_{16/17}$

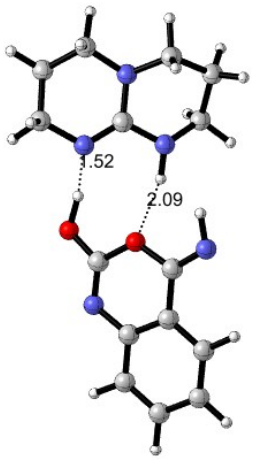


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.124121	-1.478900	0.004285
2	1	0	0.189283	1.900614	-1.457359
3	8	0	0.482251	-0.194629	-0.502232
4	6	0	0.740338	-1.364545	0.122663
5	8	0	-0.386936	-2.045073	0.308771
6	7	0	1.868665	-1.803932	0.504830
7	6	0	2.965841	-0.971220	0.254424
8	6	0	4.240089	-1.408737	0.636792
9	6	0	2.831946	0.288333	-0.353587
10	6	0	5.347154	-0.602285	0.417280
11	1	0	4.329134	-2.384080	1.104747
12	6	0	3.950819	1.097535	-0.571004
13	6	0	5.207869	0.654600	-0.186650
14	1	0	6.331211	-0.950293	0.718384
15	1	0	3.805042	2.065114	-1.041632
16	1	0	6.079752	1.279182	-0.354611
17	6	0	1.494312	0.738617	-0.753405
18	7	0	1.201191	1.844421	-1.281317
19	6	0	-2.324200	0.798844	1.954757
20	6	0	-1.250365	1.830963	1.649645
21	6	0	-1.663025	2.617301	0.407574
22	7	0	-2.660584	0.041434	0.753779
23	6	0	-2.390896	0.585474	-0.494253

24	7	0	-1.902703	1.748248	-0.736471
25	6	0	-3.660921	-1.011381	0.931786
26	6	0	-4.466919	-1.208673	-0.343412
27	6	0	-3.508276	-1.406226	-1.508106
28	7	0	-2.539692	-0.311350	-1.546305
29	1	0	-3.228553	1.294494	2.343299
30	1	0	-1.984935	0.085123	2.716247
31	1	0	-0.292714	1.330945	1.462891
32	1	0	-1.120009	2.491169	2.513199
33	1	0	-0.880052	3.332925	0.135150
34	1	0	-3.171893	-1.951910	1.229183
35	1	0	-4.321109	-0.716174	1.757814
36	1	0	-5.088011	-0.323419	-0.525902
37	1	0	-5.126914	-2.074890	-0.238555
38	1	0	-2.989363	-2.369645	-1.400121
39	1	0	-4.048898	-1.435124	-2.458717
40	1	0	-2.567124	3.206520	0.626492
41	1	0	-2.403978	0.152606	-2.435744

TBD-**17**

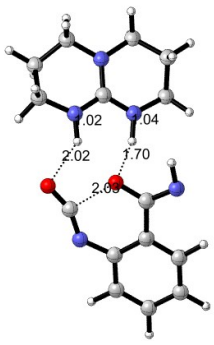


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.588566	-1.670062	0.271765
2	1	0	-0.441443	1.968354	-1.077954
3	8	0	-0.960928	-0.124257	-0.186460
4	6	0	-1.358907	-1.353918	0.296979
5	8	0	-0.335174	-2.116002	0.532506
6	7	0	-2.571418	-1.701016	0.502091
7	6	0	-3.559486	-0.760952	0.223155
8	6	0	-4.900871	-1.107415	0.449061
9	6	0	-3.271781	0.520266	-0.275902
10	6	0	-5.911369	-0.197123	0.182697
11	1	0	-5.113119	-2.099669	0.834646
12	6	0	-4.295616	1.435489	-0.545124
13	6	0	-5.614971	1.080212	-0.315748

14	1	0	-6.945478	-0.477761	0.363123
15	1	0	-4.026721	2.413477	-0.932831
16	1	0	-6.413973	1.785706	-0.521088
17	6	0	-1.873208	0.870295	-0.516250
18	7	0	-1.459410	1.973824	-0.979363
19	6	0	4.751910	-0.707467	-0.600172
20	6	0	4.315860	-2.098236	-0.165250
21	6	0	2.859037	-2.305748	-0.564236
22	7	0	3.842825	0.288461	-0.044432
23	6	0	2.512267	-0.047424	0.082042
24	7	0	2.004452	-1.227121	-0.079846
25	6	0	4.121719	1.682367	-0.390113
26	6	0	3.527036	2.648475	0.644262
27	6	0	2.294752	2.019560	1.311389
28	7	0	1.708254	1.021645	0.418969
29	1	0	4.762305	-0.639429	-1.700388
30	1	0	5.760828	-0.476559	-0.242092
31	1	0	4.417297	-2.187969	0.922561
32	1	0	4.959124	-2.852673	-0.628627
33	1	0	2.474114	-3.243912	-0.152754
34	1	0	5.208127	1.792538	-0.445339
35	1	0	3.715366	1.899253	-1.388766
36	1	0	3.259919	3.581588	0.139452
37	1	0	4.267547	2.887987	1.412985
38	1	0	2.581608	1.556454	2.265578
39	1	0	1.531340	2.772012	1.519072
40	1	0	2.773885	-2.379905	-1.657763
41	1	0	0.758385	0.731809	0.627373

TBD-$\mathbf{TS_{17/18}}$

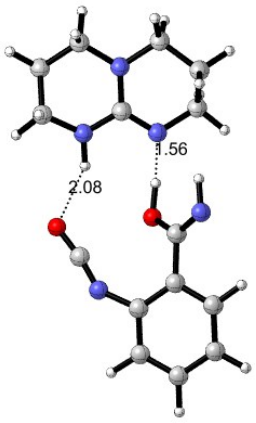


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.986277	-1.213830	0.564540
2	1	0	0.501620	1.907420	1.673531
3	8	0	0.793600	-0.178259	0.551844

4	6	0	1.398302	-2.023294	-0.033569
5	8	0	0.378914	-2.623433	0.082458
6	7	0	2.589890	-1.899860	-0.311110
7	6	0	3.435486	-0.787182	-0.250601
8	6	0	4.742247	-0.994285	-0.714499
9	6	0	3.066941	0.474573	0.248441
10	6	0	5.675913	0.031016	-0.689718
11	1	0	4.997448	-1.980927	-1.088839
12	6	0	4.026787	1.493129	0.273678
13	6	0	5.318416	1.286137	-0.191435
14	1	0	6.683195	-0.148789	-1.055440
15	1	0	3.719236	2.453250	0.675204
16	1	0	6.043897	2.093890	-0.162490
17	6	0	1.687758	0.760575	0.756661
18	7	0	1.464928	1.898627	1.327642
19	6	0	-4.706982	-0.740641	-0.110435
20	6	0	-4.049128	-2.097548	-0.321477
21	6	0	-2.864704	-2.234448	0.624643
22	7	0	-3.722005	0.335930	-0.206002
23	6	0	-2.412377	0.109718	0.030454
24	7	0	-1.996263	-1.080398	0.467173
25	6	0	-4.210906	1.661500	-0.586626
26	6	0	-3.234941	2.751899	-0.165020
27	6	0	-1.836929	2.391535	-0.648115
28	7	0	-1.505108	1.066158	-0.158779
29	1	0	-5.205822	-0.695884	0.867900
30	1	0	-5.464292	-0.557204	-0.880177
31	1	0	-3.701788	-2.180609	-1.357358
32	1	0	-4.779196	-2.891149	-0.141249
33	1	0	-2.266246	-3.119566	0.398086
34	1	0	-4.377592	1.688269	-1.672670
35	1	0	-5.180554	1.804753	-0.097380
36	1	0	-3.230334	2.843922	0.926722
37	1	0	-3.555138	3.708924	-0.585861
38	1	0	-1.790353	2.418425	-1.745210
39	1	0	-1.085389	3.084511	-0.262625
40	1	0	-3.210271	-2.310018	1.663885
41	1	0	-0.527625	0.768860	0.038274

TBD-**18**

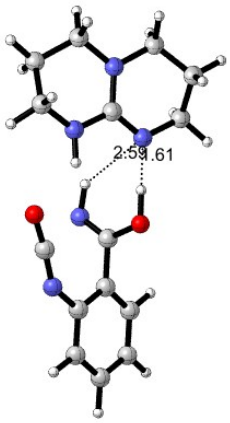


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.090962	1.456586	0.309421
2	1	0	0.191561	-2.028075	-0.697689
3	8	0	0.886001	-0.177433	0.733888
4	6	0	1.587718	2.229365	0.331314
5	8	0	0.532941	2.747258	0.427812
6	7	0	2.720515	1.858607	0.225871
7	6	0	3.546621	0.745338	0.056531
8	6	0	4.922099	0.994795	0.038544
9	6	0	3.059635	-0.559160	-0.138651
10	6	0	5.822555	-0.041032	-0.172077
11	1	0	5.261471	2.015128	0.185057
12	6	0	3.984563	-1.581625	-0.370646
13	6	0	5.352603	-1.336677	-0.383632
14	1	0	6.888522	0.166312	-0.177818
15	1	0	3.591435	-2.578894	-0.539706
16	1	0	6.048586	-2.151718	-0.556691
17	6	0	1.609163	-0.923444	-0.110085
18	7	0	1.196748	-1.893333	-0.831611
19	6	0	-4.717249	0.663842	-0.571423
20	6	0	-4.283439	2.084011	-0.240911
21	6	0	-2.824813	2.252152	-0.640626
22	7	0	-3.763262	-0.327937	-0.087700
23	6	0	-2.462134	-0.037252	0.227991
24	7	0	-2.051857	1.249722	0.060028
25	6	0	-4.240491	-1.707744	-0.123104
26	6	0	-3.086267	-2.697790	-0.074023
27	6	0	-2.098907	-2.239910	0.994832
28	7	0	-1.609996	-0.905863	0.701876
29	1	0	-4.837487	0.549841	-1.660265
30	1	0	-5.689577	0.443119	-0.112787
31	1	0	-4.384806	2.268936	0.833965
32	1	0	-4.923161	2.792666	-0.775452
33	1	0	-2.439261	3.232476	-0.351057

34	1	0	-4.925073	-1.871360	0.721835
35	1	0	-4.822289	-1.838607	-1.045088
36	1	0	-2.575315	-2.725133	-1.044001
37	1	0	-3.472710	-3.700574	0.133357
38	1	0	-2.583990	-2.266709	1.983775
39	1	0	-1.239329	-2.917087	1.046778
40	1	0	-2.717869	2.156572	-1.732250
41	1	0	-0.106261	-0.499658	0.761563

TBD-**TS$_{18/19}$**

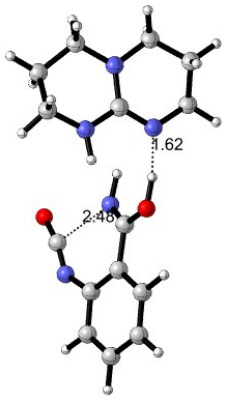


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.505973	-1.491425	-0.070820
2	6	0	-3.657415	-2.498689	-0.830966
3	6	0	-2.260907	-2.514938	-0.220599
4	7	0	-3.791176	-0.231611	0.111689
5	6	0	-2.435073	-0.162560	-0.070083
6	7	0	-1.660055	-1.193539	-0.254949
7	6	0	-4.640778	0.928064	0.360664
8	6	0	-3.842546	2.131811	0.836133
9	6	0	-2.632864	2.301603	-0.069647
10	7	0	-1.859371	1.077897	-0.000745
11	1	0	-4.794709	-1.891799	0.912117
12	1	0	-5.430948	-1.272478	-0.619771
13	1	0	-3.585142	-2.204005	-1.884354
14	1	0	-4.128196	-3.485719	-0.784322
15	1	0	-1.605755	-3.199429	-0.768272
16	1	0	-5.188923	1.178298	-0.561228
17	1	0	-5.386094	0.639304	1.112764
18	1	0	-3.498993	1.976532	1.864507
19	1	0	-4.478541	3.021656	0.815280
20	1	0	-2.957175	2.523061	-1.098961
21	1	0	-1.989814	3.119200	0.263552
22	1	0	-2.316893	-2.884822	0.815684
23	1	0	-0.069326	-1.111403	-0.516828

24	1	0	-0.896632	1.126443	-0.312544
25	1	0	0.018398	-0.258884	1.487085
26	8	0	0.950203	-1.073177	-0.658037
27	6	0	1.726897	2.127381	-0.522833
28	8	0	0.646308	2.592118	-0.585964
29	7	0	2.873070	1.771296	-0.527998
30	6	0	3.647935	0.650098	-0.204313
31	6	0	5.030267	0.731552	-0.362515
32	6	0	3.047699	-0.526023	0.261157
33	6	0	5.823502	-0.369308	-0.054974
34	1	0	5.463364	1.658179	-0.725176
35	6	0	3.854985	-1.619632	0.561052
36	6	0	5.237966	-1.546658	0.407681
37	1	0	6.900571	-0.305025	-0.176865
38	1	0	3.388269	-2.531049	0.923829
39	1	0	5.855347	-2.405979	0.650635
40	6	0	1.560291	-0.588663	0.427802
41	7	0	1.038272	-0.161085	1.510353

TBD-**19**

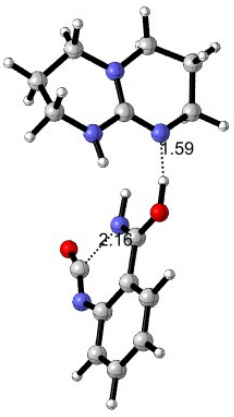


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.676677	-0.713357	-0.786422
2	6	0	4.091903	-2.098509	-1.016849
3	6	0	2.626573	-1.949409	-1.409668
4	7	0	3.795542	0.095509	0.051475
5	6	0	2.490509	-0.267512	0.245509
6	7	0	1.883790	-1.229168	-0.391112
7	6	0	4.435615	1.218965	0.725564
8	6	0	3.415789	2.199070	1.283703
9	6	0	2.363207	1.420160	2.057317
10	7	0	1.763458	0.465268	1.147696
11	1	0	4.841649	-0.198305	-1.744011
12	1	0	5.647413	-0.782123	-0.278948
13	1	0	4.158072	-2.687827	-0.094867

14	1	0	4.664420	-2.615086	-1.793399
15	1	0	2.159608	-2.929453	-1.542990
16	1	0	5.080606	0.839883	1.533729
17	1	0	5.086616	1.717523	-0.003415
18	1	0	2.928803	2.743680	0.467797
19	1	0	3.920226	2.922721	1.930617
20	1	0	2.822271	0.925030	2.927569
21	1	0	1.573919	2.082042	2.422012
22	1	0	2.556936	-1.427331	-2.377158
23	1	0	0.854611	0.076976	1.369827
24	1	0	0.327377	-1.472510	-0.019632
25	1	0	0.072009	0.288283	-1.210514
26	8	0	-0.644174	-1.498875	0.313153
27	6	0	-2.501108	2.285533	-1.277452
28	8	0	-1.805704	3.072857	-1.794162
29	7	0	-3.406831	1.672594	-0.757194
30	6	0	-3.723731	0.455070	-0.169765
31	6	0	-5.068438	0.304618	0.195371
32	6	0	-2.813643	-0.591223	0.096766
33	6	0	-5.522008	-0.854813	0.807408
34	1	0	-5.742927	1.127605	-0.017967
35	6	0	-3.293732	-1.747766	0.725215
36	6	0	-4.629671	-1.891884	1.076193
37	1	0	-6.570720	-0.946065	1.075315
38	1	0	-2.584529	-2.542162	0.928903
39	1	0	-4.970746	-2.804581	1.555038
40	6	0	-1.371462	-0.530834	-0.264714
41	7	0	-0.933882	0.375969	-1.052136

TBD-**TS**$_{19/20}$

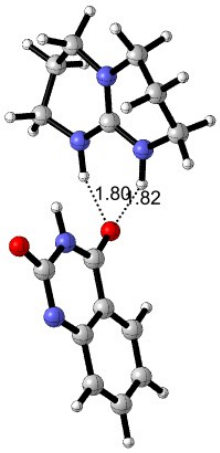


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.615346	-0.375295	-0.900526
2	6	0	4.089585	-1.682986	-1.472527
3	6	0	2.610268	-1.514483	-1.799096

4	7	0	3.721724	0.141612	0.132388
5	6	0	2.438257	-0.316847	0.236449
6	7	0	1.859269	-1.109078	-0.623674
7	6	0	4.330320	1.077676	1.072374
8	6	0	3.285207	1.826520	1.883990
9	6	0	2.281399	0.822955	2.429593
10	7	0	1.698894	0.122806	1.302701
11	1	0	4.729257	0.377650	-1.693669
12	1	0	5.601755	-0.521990	-0.442880
13	1	0	4.205669	-2.484027	-0.733202
14	1	0	4.667190	-1.954132	-2.361452
15	1	0	2.185948	-2.452875	-2.167307
16	1	0	5.009611	0.527609	1.742024
17	1	0	4.942062	1.779846	0.492620
18	1	0	2.760355	2.549542	1.250584
19	1	0	3.775740	2.369879	2.696739
20	1	0	2.778729	0.131461	3.127770
21	1	0	1.475243	1.326301	2.968469
22	1	0	2.493315	-0.772292	-2.604647
23	1	0	0.808889	-0.346359	1.421177
24	1	0	0.343478	-1.464022	-0.307841
25	1	0	0.036627	0.465370	-1.257041
26	8	0	-0.629555	-1.559187	0.036363
27	6	0	-2.324995	2.132211	-1.349425
28	8	0	-1.662549	2.921882	-1.912841
29	7	0	-3.352924	1.684380	-0.828165
30	6	0	-3.669881	0.499283	-0.183332
31	6	0	-5.001439	0.385433	0.247918
32	6	0	-2.783681	-0.570723	0.073248
33	6	0	-5.449545	-0.748120	0.907887
34	1	0	-5.667455	1.217503	0.042922
35	6	0	-3.254758	-1.707669	0.743281
36	6	0	-4.574036	-1.807423	1.159853
37	1	0	-6.486415	-0.807148	1.226955
38	1	0	-2.555095	-2.516373	0.925141
39	1	0	-4.918469	-2.699115	1.674324
40	6	0	-1.368788	-0.517077	-0.346448
41	7	0	-0.953984	0.496120	-1.013008

TBD-**20**

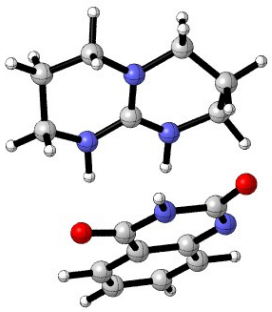


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.827286	-0.346495	-0.338200
2	6	0	4.507001	-1.825753	-0.179139
3	6	0	3.189369	-2.120444	-0.883730
4	7	0	3.676107	0.490337	-0.003692
5	6	0	2.416202	-0.007368	0.050821
6	7	0	2.159282	-1.252833	-0.345141
7	6	0	3.970448	1.902336	0.239946
8	6	0	2.710995	2.756514	0.199602
9	6	0	1.631996	2.071989	1.028867
10	7	0	1.410747	0.738889	0.505118
11	1	0	5.139983	-0.128957	-1.369530
12	1	0	5.650704	-0.054782	0.324734
13	1	0	4.413342	-2.077473	0.882976
14	1	0	5.321465	-2.420933	-0.601864
15	1	0	2.866934	-3.150840	-0.719605
16	1	0	4.467048	1.997028	1.215936
17	1	0	4.684150	2.229333	-0.526100
18	1	0	2.358610	2.860888	-0.832494
19	1	0	2.937320	3.753903	0.587335
20	1	0	1.934388	2.026737	2.084580
21	1	0	0.681826	2.609093	0.980366
22	1	0	3.294335	-1.968774	-1.967008
23	1	0	0.422125	0.385038	0.326738
24	1	0	1.215891	-1.652742	-0.098950
25	1	0	-2.478095	-3.143582	0.541792
26	8	0	-4.736186	-2.117848	0.378483
27	6	0	-1.203492	-1.560390	0.230970
28	8	0	-0.209628	-2.316779	0.360784
29	7	0	-1.112939	-0.250984	-0.011547
30	6	0	-2.267476	0.481042	-0.161931
31	6	0	-2.174356	1.859436	-0.457722
32	6	0	-3.559690	-0.072723	-0.042389
33	6	0	-3.311766	2.631082	-0.609245

34	1	0	-1.185596	2.294065	-0.584646
35	6	0	-4.705529	0.716258	-0.196878
36	6	0	-4.592182	2.067052	-0.476533
37	1	0	-3.211997	3.688811	-0.840256
38	1	0	-5.673112	0.233565	-0.090808
39	1	0	-5.477947	2.682679	-0.597094
40	6	0	-3.686314	-1.507639	0.245258
41	7	0	-2.463170	-2.147614	0.351200

TBD-**$TS_{20/21}$**

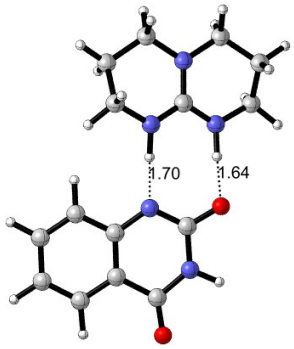


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.480714	-0.992536	0.099855
2	6	0	-3.035606	-2.409135	-0.228952
3	6	0	-1.553973	-2.549523	0.077035
4	7	0	-2.579051	0.005726	-0.482063
5	6	0	-1.318852	-0.282530	-0.832646
6	7	0	-0.840785	-1.533813	-0.694500
7	6	0	-3.102268	1.371902	-0.602785
8	6	0	-1.984224	2.393472	-0.482303
9	6	0	-0.885014	2.071060	-1.481498
10	7	0	-0.538112	0.649005	-1.386971
11	1	0	-3.520430	-0.837985	1.186192
12	1	0	-4.479491	-0.798321	-0.304888
13	1	0	-3.217509	-2.622609	-1.288068
14	1	0	-3.616889	-3.117896	0.366799
15	1	0	-1.172265	-3.523253	-0.236495
16	1	0	-3.635299	1.464349	-1.559359
17	1	0	-3.830206	1.503121	0.203451
18	1	0	-1.568412	2.394408	0.531477
19	1	0	-2.379468	3.393539	-0.680922
20	1	0	-1.200625	2.291137	-2.508593
21	1	0	0.021774	2.632808	-1.241711
22	1	0	-1.336562	-2.428180	1.145212
23	1	0	0.445575	0.413538	-1.488812

24	1	0	0.168110	-1.636042	-0.771384
25	1	0	-0.150756	0.301723	2.799985
26	8	0	0.746986	-1.898390	2.038269
27	6	0	0.722257	1.686532	1.522468
28	8	0	0.044158	2.578992	2.039073
29	7	0	1.598245	1.841943	0.515145
30	6	0	2.222888	0.742062	0.026198
31	6	0	3.096222	0.895179	-1.089966
32	6	0	2.023890	-0.587642	0.491764
33	6	0	3.714384	-0.192804	-1.672916
34	1	0	3.261982	1.903877	-1.458429
35	6	0	2.672223	-1.683860	-0.102215
36	6	0	3.513184	-1.500978	-1.184544
37	1	0	4.375662	-0.035392	-2.521625
38	1	0	2.493359	-2.670316	0.320688
39	1	0	4.018007	-2.343913	-1.645283
40	6	0	1.069852	-0.798519	1.582384
41	7	0	0.495243	0.364928	2.020069

TBD-**21**



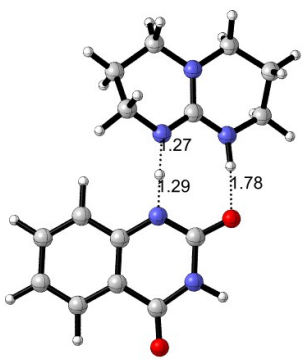
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.827286	-0.346495	-0.338200
2	6	0	4.507001	-1.825753	-0.179139
3	6	0	3.189369	-2.120444	-0.883730
4	7	0	3.676107	0.490337	-0.003692
5	6	0	2.416202	-0.007368	0.050821
6	7	0	2.159282	-1.252833	-0.345141
7	6	0	3.970448	1.902336	0.239946
8	6	0	2.710995	2.756514	0.199602
9	6	0	1.631996	2.071989	1.028867
10	7	0	1.410747	0.738889	0.505118
11	1	0	5.139983	-0.128957	-1.369530
12	1	0	5.650704	-0.054782	0.324734
13	1	0	4.413342	-2.077473	0.882976

14	1	0	5.321465	-2.420933	-0.601864
15	1	0	2.866934	-3.150840	-0.719605
16	1	0	4.467048	1.997028	1.215936
17	1	0	4.684150	2.229333	-0.526100
18	1	0	2.358610	2.860888	-0.832494
19	1	0	2.937320	3.753903	0.587335
20	1	0	1.934388	2.026737	2.084580
21	1	0	0.681826	2.609093	0.980366
22	1	0	3.294335	-1.968774	-1.967008
23	1	0	0.422125	0.385038	0.326738
24	1	0	1.215891	-1.652742	-0.098950
25	1	0	-2.478095	-3.143582	0.541792
26	8	0	-4.736186	-2.117848	0.378483
27	6	0	-1.203492	-1.560390	0.230970
28	8	0	-0.209628	-2.316779	0.360784
29	7	0	-1.112939	-0.250984	-0.011547
30	6	0	-2.267476	0.481042	-0.161931
31	6	0	-2.174356	1.859436	-0.457722
32	6	0	-3.559690	-0.072723	-0.042389
33	6	0	-3.311766	2.631082	-0.609245
34	1	0	-1.185596	2.294065	-0.584646
35	6	0	-4.705529	0.716258	-0.196878
36	6	0	-4.592182	2.067052	-0.476533
37	1	0	-3.211997	3.688811	-0.840256
38	1	0	-5.673112	0.233565	-0.090808
39	1	0	-5.477947	2.682679	-0.597094
40	6	0	-3.686314	-1.507639	0.245258
41	7	0	-2.463170	-2.147614	0.351200

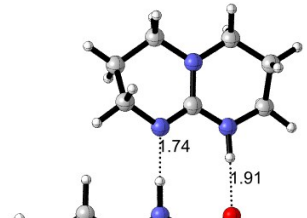
TBD-$\mathbf{TS_{21/22}}$

Standard orientation:



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.771352	-0.206317	-0.374931
2	6	0	4.551490	-1.708984	-0.287618
3	6	0	3.250900	-2.049225	-1.002977

4	7	0	3.572847	0.536692	0.001622
5	6	0	2.333890	-0.030603	0.052140
6	7	0	2.171029	-1.286736	-0.410114
7	6	0	3.783615	1.956988	0.273264
8	6	0	2.467382	2.718273	0.352737
9	6	0	1.484230	1.889019	1.172075
10	7	0	1.284974	0.601780	0.537304
11	1	0	5.065621	0.076580	-1.396794
12	1	0	5.581144	0.106004	0.296546
13	1	0	4.479074	-2.018898	0.760730
14	1	0	5.400536	-2.227886	-0.742366
15	1	0	3.003438	-3.108271	-0.902944
16	1	0	4.337099	2.054421	1.218303
17	1	0	4.421400	2.362319	-0.523129
18	1	0	2.055677	2.869179	-0.651739
19	1	0	2.643117	3.700896	0.801121
20	1	0	1.867665	1.762145	2.196255
21	1	0	0.511509	2.383234	1.253591
22	1	0	3.341972	-1.826512	-2.075928
23	1	0	0.122039	0.146521	0.292122
24	1	0	1.301820	-1.761211	-0.120614
25	1	0	-2.563993	-3.157089	0.582537
26	8	0	-4.755595	-2.017440	0.330062
27	6	0	-1.196352	-1.651764	0.320565
28	8	0	-0.239140	-2.424560	0.488511
29	7	0	-1.056695	-0.335801	0.070397
30	6	0	-2.158966	0.463287	-0.149539
31	6	0	-1.982169	1.824556	-0.468380
32	6	0	-3.472112	-0.037392	-0.075188
33	6	0	-3.079983	2.640350	-0.681987
34	1	0	-0.971599	2.213510	-0.564556
35	6	0	-4.573724	0.796727	-0.293085
36	6	0	-4.387019	2.135606	-0.592461
37	1	0	-2.923332	3.686989	-0.929747
38	1	0	-5.565356	0.359141	-0.220346
39	1	0	-5.237915	2.786954	-0.763911
40	6	0	-3.674730	-1.462510	0.228698
41	7	0	-2.489136	-2.164518	0.386849



TBD-**22**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.848095	-0.320033	-0.360346
2	6	0	4.572457	-1.803209	-0.171503
3	6	0	3.257297	-2.133199	-0.863313
4	7	0	3.692095	0.492418	-0.006491
5	6	0	2.410936	-0.002045	0.072160
6	7	0	2.211432	-1.289988	-0.325431
7	6	0	3.964572	1.922847	0.093214
8	6	0	2.677911	2.733673	0.152791
9	6	0	1.692687	1.993706	1.053542
10	7	0	1.390689	0.684066	0.510043
11	1	0	5.132092	-0.120560	-1.406255
12	1	0	5.688189	0.001486	0.269313
13	1	0	4.490855	-2.038645	0.895544
14	1	0	5.398436	-2.385103	-0.592305
15	1	0	2.967352	-3.173467	-0.696565
16	1	0	4.570477	2.102490	0.993411
17	1	0	4.573099	2.219103	-0.772799
18	1	0	2.240556	2.824868	-0.848223
19	1	0	2.897335	3.740865	0.521859
20	1	0	2.119783	1.908610	2.066993
21	1	0	0.758368	2.555916	1.155764
22	1	0	3.363003	-1.987657	-1.949207
23	1	0	-0.205250	0.052749	0.250063
24	1	0	1.334810	-1.715270	-0.021407
25	1	0	-2.702098	-3.177300	0.445587
26	8	0	-4.865037	-2.003439	0.157753
27	6	0	-1.306280	-1.690074	0.320578
28	8	0	-0.354393	-2.448510	0.486760
29	7	0	-1.179384	-0.350118	0.133658
30	6	0	-2.255847	0.493875	-0.076684
31	6	0	-2.044396	1.863636	-0.297084
32	6	0	-3.564172	-0.010414	-0.079040
33	6	0	-3.131351	2.697900	-0.502885

34	1	0	-1.027339	2.245115	-0.313909
35	6	0	-4.651303	0.843655	-0.288618
36	6	0	-4.441664	2.196765	-0.497939
37	1	0	-2.960742	3.757029	-0.674597
38	1	0	-5.647959	0.411965	-0.281999
39	1	0	-5.281244	2.864323	-0.661701
40	6	0	-3.781467	-1.451862	0.134269
41	7	0	-2.606134	-2.176698	0.306715

S5: Reference 13 details.

13. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.