SUPPORTING INFORMATION II FOR:

ANRORC type rearrangement/intermolecular cyclocondensation cascade of 5,6-dicyano-3-(2-oxo-2-ethyl)pyrazin-2(1*H*)-ones with hydrazine hydrate for the synthesis of 2-(pyrazol-3-yl)imidazo[4,5-*d*]pyridazines

Vakhid A. Mamedov,*[a] Venera R. Galimullina,[a] Zheng-Wang Qu,*[b] Hui Zhu,[b] Victor V. Syakaev,[a] Dariya V. Nikolaeva,[a] Il'dar Kh. Rizvanov,[a] Aidar T. Gubaidullin,[a] Oleg G. Sinyashin,[a] and Stefan Grimme[b]

[a] A.E. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Arbuzov Street 8, 420088 Kazan, Russian Federation
E-mail: mamedov@iopc.ru

[b] Mulliken Center for Theoretical Chemistry University of Bonn Beringstr. 4, 53115 Bonn, Germany
E-mail: qu@thch.uni-bonn.de

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Computational Methods

All DFT calculations are performed with the TURBOMOLE 7.4 suite of programs.[1] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO level, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3] and the def2-TZVP basis set,[4] using the Conductor-like Screening Model (COSMO)[5] for butanol solvent (dielectric constant $\varepsilon = 17.5$ and radium $R_{solv} = 3.31$ Å). The density-fitting RI-J approach[6] is used to accelerate the calculations. The optimized structures are characterized by frequency analysis (no imaginary frequency for true minima and only one imaginary frequency for transition states) to provide thermal free-energy corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[7]

More accurate solvation free energies in butanol are computed with the COSMO-RS model[8] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm package[9] based on the TPSS-D3 optimized structures, corrected by +1.89 kcal/mol to account for the 1 mol/L reference concentration in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at both TPSS-D3[2] and hybrid-meta-GGA PW6B95-D3[10] levels are performed using the larger def2-QZVP[4] basis set. Final reaction free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. As expected, the reaction energy results from both DFT functionals are in good mutual agreement (-0.4 ± 1.7 kcal/mol, mean ± standard deviation) but somewhat higher reaction barriers (4.9 ± 3.1 kcal/mol) are found at the PW6B95-D3 level compared to the TPSS-D3 results. In our discussion, the more reliable PW6B95-D3 + COSMO-RS free energies (in kcal/mol, at 298.15 K and 1 mol/L concentration) are used unless specified otherwise. The applied DFT methods in combination with the large AO basis set provide usually accurate electronic energies leading to errors for chemical energies (including barriers) on the order of typically 1-2 kcal/mol. This has been tested thoroughly for the huge data base GMTKN55[11] which is the common standard in the field of DFT benchmarking.

[1] TURBOMOLE V7.4, 2019, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.
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[11] L. Goerigk, A. Hansen, C. Bauer, S. Ehrlich, A. Najibi, S. Grimme, *Phys. Chem. Chem. Phys.*, 2017, **19**, 32184−32215.

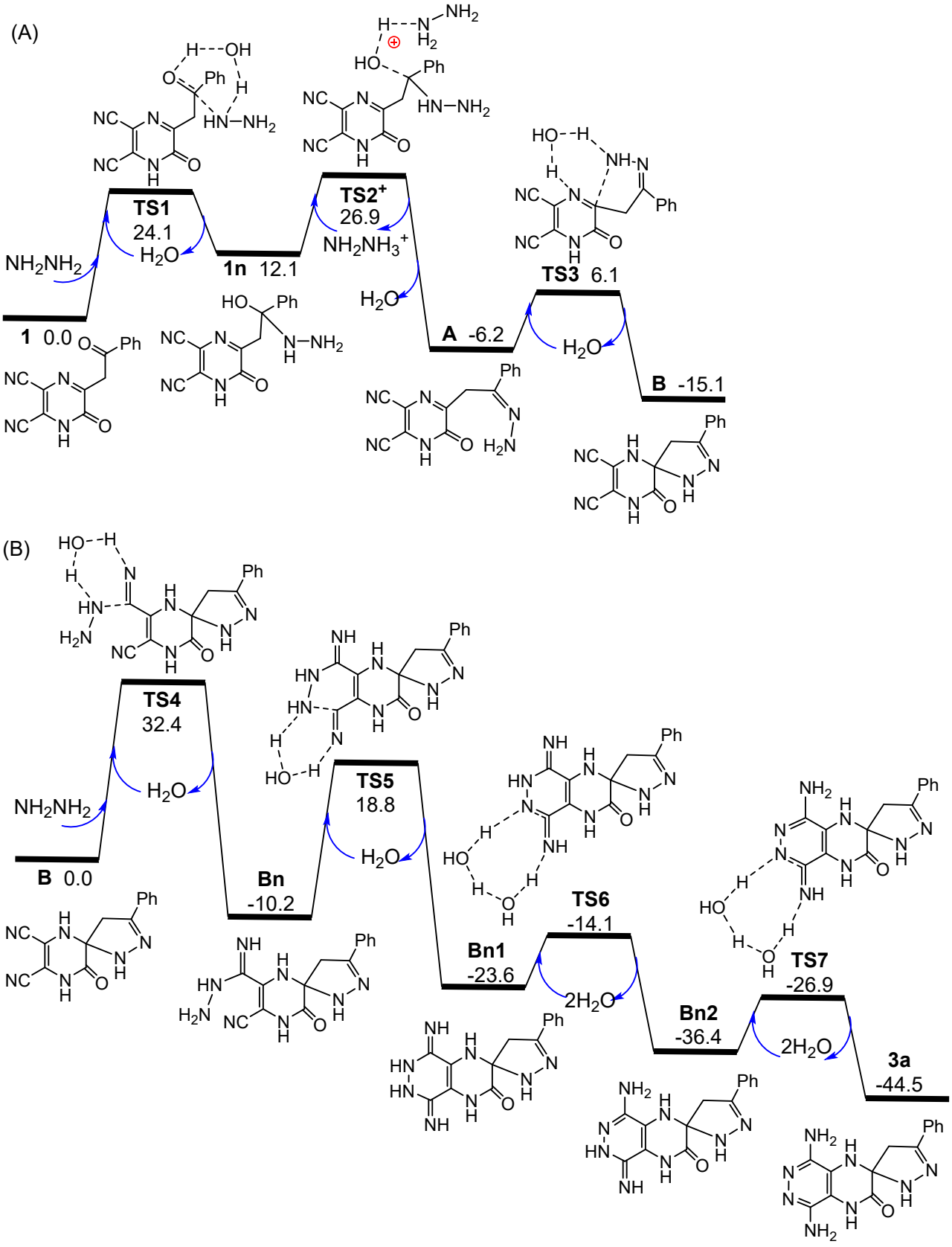

Fig. S1 DFT-computed reaction free energy profile (at 298 K and 1 M concentration) at the PW6B95-D3/def2-QZVP + COSMO-RS // TPSS-D3/def2-TZVP + COSMO level in *n*-BuOH solution: (A) condensation of pyrazin-2(1*H*)-one-5,6-dicarbonitrile with the N_2H_4; (B) addition of the second N_2H_4 to the 5′-phenyl-1,4′-dihydrospiro[pyrazine-2,3′-pyrazol]-3(4*H*)-one-5,6-dicarbonitrile.

Table S1. DFT-computed energies for the H_2SO_4-induced rearrangement of **1**. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in butanol solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels. Each structure is labeled either by its molecular formula or a specific name in bold, with singly charged cation and anion species indicated by the + and – superscripts, respectively. Transition structures (with only one imaginary frequency) are indicated by the "**TS**" prefix. See also main-text **Figure 1** for labelings.

Reactions in BuOH	ImF cm^{-1}	ZPE kcal/mol	Hc kcal/mol	Gc kcal/mol	Hsol kcal/mol	Gsol kcal/mol	TPSS Eh	PW6B95 Eh	Gp kcal/mol	ΔEt kcal/mol	ΔEp kcal/mol	ΔG_P *kcal/mol*	ΔG_T kcal/mol
H^+ exists as $NH_2NH_3^+$ in BuOH solution													
$N_2H_4 + H_2SO_4$	0	56.09	62.88	24.11	-55.05	-25.56	-812.46288	-813.16600	-813.16230	0.00	0.00	*0.00*	0.00
$NH_2NH_3^+ + HSO_4^-$	0	58.92	65.28	26.84	-177.28	-141.98	-812.30172	-813.00595	-813.18342	101.13	100.43	*-13.25*	-12.55
$N_2H_4 + HSO_4^-$	0	48.78	55.39	16.83	-91.32	-70.18	-811.95255	-812.65747	-812.73646	0.00	0.00	*0.00*	0.00
$NH_2NH_3^+ + SO_4^{2-}$	0	51.93	57.83	20.25	-410.49	-325.93	-811.56663	-812.27364	-812.75475	242.17	240.86	*-11.48*	-10.16
$H_2SO_4 + NH_2NH_3^+$	0	66.24	72.77	34.12	-141.01	-97.37	-812.81205	-813.51448	-813.60926	0.00	0.00	*0.00*	0.00
$HSO_4^- + NH_3NH_3^{2+}$	0	67.87	74.23	35.66	-398.60	-338.68	-812.39811	-813.09994	-813.57681	259.75	260.13	*20.36*	19.98
$N_2H_4 + H_2O$	0	45.34	50.69	19.96	-27.47	-11.86	-188.41004	-188.59775	-188.57880	0.00	0.00	*0.00*	0.00
$N_2H_4.OH_2$	0	47.20	52.29	28.62	-28.06	-14.39	-188.41861	-188.60696	-188.58127	-5.38	-5.78	*-1.55*	-1.14
H_2O-aided first N_2H_4 addition													
1 + N_2H_4 + H_2O	0	166.59	183.13	113.94	-55.08	-31.56	-1096.71684	-1097.87287	-1097.73255	0.00	0.00	*0.00*	0.00
TS1	517i	169.05	182.94	138.68	-47.49	-30.67	-1096.72244	-1097.86937	-1097.69423	-3.51	2.19	*24.05*	18.34
TS1a - H_2O	713i	170.70	183.54	151.02	-40.97	-28.56	-1096.73637	-1097.87950	-1097.68433	-12.26	-4.16	*30.25*	22.16
1n + H_2O	0	169.70	184.89	130.27	-47.05	-28.03	-1096.72596	-1097.88217	-1097.71322	-5.73	-5.84	*12.13*	12.24
TS2a	993i	166.58	180.83	136.76	-44.66	-30.45	-1096.70212	-1097.84381	-1097.67138	9.24	18.23	*38.38*	29.39
A + $2H_2O$	0	166.08	182.52	116.40	-51.51	-29.29	-1096.73459	-1097.89023	-1097.74239	-11.14	-10.90	*-6.18*	-6.42
1n + $NH_2NH_3^+$	0	199.23	214.77	156.46	-137.84	-102.39	-1132.53841	-1133.72875	-1133.63655	0.00	0.00	*12.13*	12.24
TS2$^+$	475i	195.55	211.58	163.15	-90.35	-67.90	-1132.58539	-1133.76781	-1133.61300	-29.48	-24.51	*26.91*	22.05
1 + N_2H_4	0	153.61	167.78	112.05	-43.75	-26.91	-1020.24345	-1021.32304	-1021.18133	0.00	0.00	*0.00*	0.00
TS1b	1541i	153.04	166.01	124.01	-36.86	-24.63	-1020.21263	-1021.28657	-1021.12518	19.35	22.89	*35.24*	31.69
1n	0	156.73	169.54	128.38	-35.73	-23.38	-1020.25258	-1021.33234	-1021.16201	-5.73	-5.84	*12.13*	12.24

TS2b	540i	151.87	164.74	123.25	-32.52	-21.81	-1020.17257	-1021.23780	-1021.07314	44.48	53.49	*67.89*	58.88
A + H_2O	0	153.10	167.17	114.51	-40.19	-24.64	-1020.26120	-1021.34041	-1021.19117	-11.14	-10.90	*-6.18*	-6.42
A	0	140.13	151.82	112.61	-28.86	-19.99	-943.78782	-944.79058	-944.63996	0.00	0.00	*-6.18*	-6.42
TS3a	1719i	136.69	148.14	109.09	-33.51	-23.75	-943.73888	-944.73941	-944.60039	30.71	32.11	*18.65*	17.01
TS3 - H_2O	1250i	138.14	148.34	120.75	-32.07	-23.14	-943.77895	-944.77603	-944.62047	5.56	9.13	*6.05*	2.24
B	0	139.94	151.55	112.54	-34.32	-23.16	-943.79245	-944.79968	-944.65424	-2.91	-5.71	*-15.14*	-12.58
B + NH_2NH_2	0	172.30	186.89	130.61	-50.46	-30.36	-1055.72911	-1056.84761	-1056.68183	0.00	0.00	*0.00*	0.00
TS4b	1700i	171.78	185.18	142.34	-42.09	-27.30	-1055.68235	-1056.79513	-1056.60879	29.35	32.93	*45.83*	42.25
TS4	1196i	174.19	186.44	154.77	-36.55	-26.98	-1055.72624	-1056.83385	-1056.63021	1.80	8.63	*32.40*	25.57
TS4a -2H_2O	1028i	176.31	187.54	166.31	-32.90	-26.12	-1055.74343	-1056.84655	-1056.62615	-8.99	0.66	*34.94*	25.29
Bn	0	175.41	188.79	146.31	-36.83	-25.15	-1055.77393	-1056.89421	-1056.69813	-28.12	-29.25	*-10.23*	-9.11
TS5	1255i	175.29	186.49	157.12	-45.60	-31.40	-1055.74508	-1056.85226	-1056.65191	-10.02	-2.92	*18.78*	11.68
Bn1	0	177.04	189.37	149.23	-43.80	-29.16	-1055.79449	-1056.91375	-1056.71940	-41.02	-41.51	*-23.58*	-23.10
TS6a	1054i	174.84	186.38	156.28	-39.99	-28.85	-1055.79431	-1056.90533	-1056.70226	-40.91	-36.23	*-12.82*	-17.51
TS6 -2H_2O	409i	176.71	187.41	167.59	-37.88	-28.69	-1055.81525	-1056.92260	-1056.70425	-54.05	-47.06	*-14.07*	-21.06
Bn2	0	177.60	189.85	149.92	-42.55	-27.98	-1055.81722	-1056.93723	-1056.73990	-55.29	-56.24	*-36.44*	-35.49
TS7a	570i	176.11	187.40	157.96	-44.02	-32.19	-1055.81286	-1056.92517	-1056.72475	-52.56	-48.67	*-26.93*	-30.82
TS7 -2H_2O	798i	177.64	187.54	169.61	-40.58	-31.35	-1055.83366	-1056.94208	-1056.72476	-65.60	-59.28	*-26.94*	-33.26
3a	0	177.17	189.54	149.38	-45.58	-29.83	-1055.82453	-1056.94634	-1056.75281	-59.88	-61.95	*-44.54*	-42.47
3a + H_2SO_4	0	200.89	217.08	155.41	-84.48	-48.19	-1756.35075	-1758.06441	-1757.88752	0.00	0.00	*0.00*	0.00
C$^+$ + HSO_4^-	0	201.75	217.94	156.11	-179.28	-138.94	-1756.18485	-1757.89530	-1757.86192	104.11	106.12	*16.07*	14.05
C+	0	185.34	197.90	157.35	-104.11	-75.97	-1056.16896	-1057.28575	-1057.15305	0.00	0.00	*16.07*	14.05
TS8$^+$	139i	183.47	196.22	155.11	-99.78	-72.37	-1056.17102	-1057.28498	-1057.15013	-1.30	0.48	*17.90*	14.11
Dc$^+$	0	183.95	196.68	155.76	-85.29	-63.44	-1056.19639	-1057.31026	-1057.16012	-17.21	-15.38	*11.63*	7.78
TS9$^+$	448i	181.73	194.94	152.53	-88.88	-65.80	-1056.15415	-1057.26838	-1057.12715	9.29	10.90	*32.32*	28.69
D$^+$	0	185.39	198.01	157.24	-88.76	-67.32	-1056.19598	-1057.30955	-1057.16325	-16.96	-14.93	*9.67*	5.63
E$^+$	0	185.05	198.13	156.43	-99.14	-70.26	-1056.20961	-1057.33124	-1057.19090	-25.51	-28.54	*-7.68*	-6.67
TS10$^+$	292i	183.81	196.66	155.17	-102.23	-71.26	-1056.18364	-1057.30241	-1057.16568	-9.21	-10.45	*8.14*	7.37

Ec^{+}	0	185.72	198.35	157.57	-103.47	-72.34	-1056.18734	-1057.30878	-1057.16995	-11.54	-14.45	*5.47*	6.36
TS11^{+}	1557i	181.24	194.00	152.69	-100.10	-71.92	-1056.14083	-1057.25795	-1057.12621	17.65	17.45	*32.91*	31.09
F^{+} + H_2O	0	181.93	195.93	143.53	-103.85	-72.54	-1056.21884	-1057.34314	-1057.22398	-31.30	-36.01	*-28.44*	-25.75
3a	0	177.17	189.54	149.38	-45.58	-29.83	-1055.82453	-1056.94634	-1056.75281	0.00	0.00	*0.00*	0.00
Dc	0	175.66	188.69	147.08	-45.62	-30.26	-1055.80762	-1056.92886	-1056.73967	10.62	10.97	*8.25*	7.89
TS9	145i	174.05	186.97	145.34	-43.96	-29.81	-1055.77900	-1056.89919	-1056.71206	28.57	29.59	*25.57*	24.56
D	0	176.50	189.17	148.26	-40.14	-27.22	-1055.82029	-1056.94010	-1056.74420	2.66	3.91	*5.40*	4.15
E	0	177.52	190.21	149.20	-43.61	-28.76	-1055.85364	-1056.97710	-1056.78217	-18.27	-19.31	*-18.42*	-17.38
F + H_2O	0	173.56	187.47	135.24	-58.28	-35.03	-1055.83721	-1056.96480	-1056.79907	-7.95	-11.59	*-29.03*	-25.40
2 + H_2O	0	173.93	187.79	135.73	-64.82	-38.88	-1055.83329	-1056.96131	-1056.80095	-5.49	-9.39	*-30.20*	-26.30
2.H_2O	0	176.66	189.63	148.11	-55.84	-35.55	-1055.85552	-1056.98022	-1056.79783	-19.45	-21.26	*-28.25*	-26.43
1 + H_2O	0	134.23	147.79	95.87	-38.93	-24.36	-984.78018	-985.82494	-985.70496	0.00	0.00	*0.00*	0.00
1p_tsa	963i	133.16	145.43	104.84	-49.40	-29.97	-984.74349	-985.77717	-985.65484	23.02	29.98	*31.45*	24.50
1p_ts - H_2O	1165i	135.42	146.87	116.70	-37.11	-24.00	-984.78055	-985.81305	-985.66533	-0.23	7.46	*24.87*	17.18
1p + H_2O	0	134.32	147.71	96.22	-36.60	-22.41	-984.79407	-985.83522	-985.71156	-8.71	-6.45	*-4.14*	-6.41
B + H_2SO_4	0	163.67	179.09	118.57	-73.22	-41.52	-1644.31868	-1645.91776	-1645.78895	0.00	0.00	*0.00*	0.00
B^{+} + HSO_4^{-}	0	165.90	181.12	120.86	-171.25	-136.08	-1644.15835	-1645.75519	-1645.77343	100.60	102.01	*9.74*	8.33
BH^{+} + HSO_4^{-}	0	163.02	178.63	117.73	-166.43	-132.86	-1644.12775	-1645.72192	-1645.74000	119.81	122.89	*30.72*	27.64

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in butanol solution for the H_2SO_4-catalyzed rearrangement. Each structure is labeled by the specific name (See also **Table S1** and main-text **Figure 1**), followed by the number of atoms, the total energy, and the detailed atomic coordinates.

1n

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34
Energy = -1020.223386268
C     1.4840150    1.1622997   -0.2422471
O     1.7371443    2.4990965   -0.6622650
C     2.7737235    0.3534064   -0.0611668
C     0.5455321    0.5478284   -1.3598418
C     3.9579820    1.0078341    0.2983395
C     2.7858235   -1.0413185   -0.1889108
H     0.3588980    1.3711457   -2.0523129
H     1.0579336   -0.2544479   -1.8883778
C    -0.7675557    0.0654673   -0.8517645
C     5.1307594    0.2865022    0.5195075
H     3.9811009    2.0890084    0.3956735
C     3.9581457   -1.7652707    0.0408907
H     1.8793720   -1.5709792   -0.4697300
C    -1.0321930   -1.3855329   -0.8170118
N    -1.6677074    0.9769854   -0.5299188
C     5.1346026   -1.1043771    0.3935693
H     6.0418289    0.8130072    0.7894185
H     3.9492356   -2.8467287   -0.0622525
O    -0.2471388   -2.2666224   -1.1656005
N    -2.3064643   -1.7100691   -0.3608444
C    -2.8760501    0.5614037   -0.0392141
H     6.0483850   -1.6661768    0.5647505
H    -2.5359558   -2.6991491   -0.3017912
C    -3.2144611   -0.7761551    0.0623809
C    -3.8008360    1.5697246    0.3637489
C    -4.4683167   -1.2202841    0.5565075
N    -4.5476485    2.3969367    0.6938646
N    -5.4953498   -1.5807291    0.9651345
N     0.8229725    1.2809969    1.0702540
H     2.1522545    2.9653405    0.0857543
H    -0.0281063    1.8342608    0.9062344
N     0.3412698   -0.0371838    1.4512809
H     1.1615757   -0.5777117    1.7341753
H    -0.2232139    0.0895296    2.2926370
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1p_ts

```
34
Energy = -1061.224283077
C     1.6618559    0.4997508   -0.1689355
O     1.3507180    1.5863585   -0.7086457
C     3.0511098   -0.0119697   -0.3601845
C     0.7524511   -0.2678170    0.6818116
C     4.0397750    0.8944603   -0.7796971
C     3.3967051   -1.3596917   -0.1701016
H     1.1241460    1.8199091    3.0794818
H     1.1660044   -1.1668271    1.1273527
C    -0.6460842   -0.4170999    0.3697251
C     5.3463004    0.4663516   -0.9908331
H     3.7637207    1.9334476   -0.9280799
C     4.7037165   -1.7895004   -0.3933057
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H     2.6437637   -2.0835193    0.1243588
C    -1.2839480   -1.6556647    0.9057151
N    -1.3402881    0.4924259   -0.3030081
C     5.6810521   -0.8780034   -0.7985951
H     6.1057070    1.1766979   -1.3044870
H     4.9579059   -2.8361387   -0.2549927
O    -0.7102969   -2.5065531    1.5850343
N    -2.6212588   -1.7930256    0.5717654
C    -2.6564030    0.2703783   -0.5666224
H     6.7002318   -1.2138582   -0.9671305
H    -3.0881016   -2.6347688    0.9012286
C    -3.3303604   -0.8640964   -0.1487504
C    -3.3470999    1.2848224   -1.2981643
C    -4.6993567   -1.1048622   -0.4163284
N    -3.8976588    2.1215548   -1.8876394
N    -5.8247238   -1.2993235   -0.6389564
O     0.3372645    1.5635569    2.5649119
H     0.6143173    0.6680737    1.8046569
H     0.0954121    2.3413191    1.8916145
O    -0.1877085    3.1747783    0.6924212
H    -1.1342705    3.1322308    0.4782889
H     0.2658804    2.5791990    0.0123151
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1p

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28
Energy = -908.2943829115
C    -1.5591863    0.3873054    0.0001607
O    -1.0807743    1.5580884    0.0044299
C    -3.0350536    0.2080185    0.0013448
C    -0.6919042   -0.7658200   -0.0059587
C    -3.8453363    1.3568721   -0.0056894
C    -3.6477495   -1.0568564    0.0095771
H     0.5746713    1.3584156    0.0042873
H    -1.0846658   -1.7723896   -0.0123887
C     0.6750431   -0.6450512   -0.0051959
C    -5.2313909    1.2444313   -0.0052016
H    -3.3669023    2.3306582   -0.0118459
C    -5.0363888   -1.1676268    0.0101338
H    -3.0512188   -1.9624506    0.0169017
C     1.5418671   -1.8531488   -0.0113356
N     1.2828412    0.5832940    0.0013709
C    -5.8311877   -0.0191426    0.0025572
H    -5.8475288    2.1387949   -0.0107131
H    -5.4980214   -2.1504410    0.0165449
O     1.1048935   -2.9978207   -0.0185594
N     2.9009153   -1.5963350   -0.0080490
C     2.6363105    0.7648662    0.0038311
H    -6.9137814   -0.1077691    0.0028047
H     3.5126527   -2.4086366   -0.0117063
C     3.4678618   -0.3317984   -0.0006138
C     3.1427843    2.0897409    0.0108230
C     4.8757046   -0.2173190    0.0022230
N     3.5496850    3.1781514    0.0164831
N     6.0367107   -0.1376961    0.0045454
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1

28
Energy = -908.2848805536

C	1.5345224	0.2408250	0.2929482
O	0.9839146	0.5212848	1.3536065
C	3.0120827	0.2014191	0.1579765
C	0.6887596	-0.0598856	-0.9552716
C	3.7963780	0.4639608	1.2945516
C	3.6419734	-0.0807533	-1.0647344
H	0.8306676	0.7424386	-1.6856043
H	1.0300384	-1.0005170	-1.4015376
C	-0.7553411	-0.1629819	-0.5981477
C	5.1835219	0.4412449	1.2088951
H	3.2980107	0.6819604	2.2337518
C	5.0326872	-0.0995692	-1.1486597
H	3.0544370	-0.2832226	-1.9543220
C	-1.1676820	-1.3715478	0.1416475
N	-1.5758824	0.8006775	-0.9212784
C	5.8038347	0.1596530	-0.0134748
H	5.7852649	0.6422372	2.0902339
H	5.5141218	-0.3168205	-2.0972257
O	-0.4281656	-2.3030418	0.4415007
N	-2.5225561	-1.3771667	0.4818939
C	-2.8948977	0.7086852	-0.5566581
H	6.8878633	0.1425500	-0.0798433
H	-2.8634083	-2.1835438	1.0020834
C	-3.3824803	-0.3744882	0.1531130
C	-3.7579843	1.7785465	-0.9329754
C	-4.7430263	-0.4850616	0.5528459
N	-4.4603344	2.6514193	-1.2411958
N	-5.8556626	-0.5683593	0.8745980

1^{+}
29
Energy = -908.7020059463

C	1.5778406	0.3710666	0.0025952
O	1.0308709	1.4914978	0.0034801
C	3.0342431	0.2365361	0.0006598
C	0.7337496	-0.9006394	0.0037161
C	3.8198997	1.4063726	-0.0016536
C	3.6605991	-1.0242098	0.0012398
H	0.9934583	-1.5237451	-0.8633373
H	0.9915998	-1.5199038	0.8742037
C	-0.7386836	-0.7146680	0.0018039
C	5.2042597	1.3123777	-0.0032527
H	3.3280129	2.3730730	-0.0022732
C	5.0482816	-1.1107227	-0.0000619
H	3.0756454	-1.9375338	0.0027910
C	-1.6164658	-1.8979902	-0.0018633
N	-1.2565123	0.4905659	0.0033768
C	5.8195167	0.0546926	-0.0022665
H	5.8092257	2.2134207	-0.0053632
H	5.5290327	-2.0834659	0.0006296
O	-1.2123275	-3.0462413	-0.0032318
N	-2.9801730	-1.5734739	-0.0039310
C	-2.6046917	0.7644803	0.0016952
H	6.9030800	-0.0160414	-0.0030707

H -3.6300710 -2.3602678 -0.0077709
C -3.4748979 -0.3098470 -0.0020730
C -3.0287268 2.1136723 0.0039066
C -4.8850746 -0.1258579 -0.0041139
N -3.3748257 3.2221881 0.0056724
N -6.0347360 0.0276676 -0.0058311
H -0.4674849 1.2416798 0.0046288

2w
37
Energy = -1055.831770031
C -2.5855480 -0.4056904 -0.0129579
C -3.9842330 0.0174909 0.0078352
C -1.3997869 0.3162460 0.0815840
C -4.3230547 1.2932416 0.4919198
C -5.0132650 -0.8232538 -0.4517104
H -1.2929286 1.3853318 0.1838171
C -0.3625271 -0.6412365 -0.0080777
C -5.6500740 1.7141696 0.5153153
H -3.5422714 1.9505787 0.8629533
C -6.3409470 -0.4014566 -0.4204170
H -4.7808183 -1.8049113 -0.8554644
C 1.0708080 -0.3910182 0.0281124
N 1.5476525 0.8865749 0.1562161
C -6.6659716 0.8683804 0.0617589
H -5.8925074 2.7028584 0.8942275
H -7.1220299 -1.0643812 -0.7813282
N 2.0124230 -1.3627717 -0.0605393
C 2.8968599 0.7212117 0.1449281
H -7.7010192 1.1965124 0.0827907
H 6.4176023 -0.3332781 -0.0064553
C 3.1734872 -0.6506689 0.0127467
C 3.9640740 1.6667454 0.2299242
C 4.5148496 -1.0832208 -0.0376020
N 5.2254679 1.2499009 0.1592718
N 5.4317732 -0.0992642 0.0324393
N -2.1985041 -1.7096032 -0.1502208
N -0.8618520 -1.8873623 -0.1449666
H -2.7959375 -2.5245170 -0.2015961
N 3.7313040 2.9976497 0.4297864
H 4.5038685 3.6295950 0.2574140
H 2.7969034 3.3516278 0.2092145
N 4.8901927 -2.3822626 -0.0997998
H 5.8324548 -2.6268614 -0.3778747
H 4.1690675 -3.0429449 -0.3620814
O 0.8041662 3.5047229 0.0096003
H 0.9207146 2.5052924 0.0460458
H 0.5484648 3.6985244 -0.9058650

2
34
Energy = -979.3426105546
C -2.6092509 -0.4253113 -0.0099117
C -4.0117414 -0.0143300 -0.0035903
C -1.4291092 0.3103449 0.0410809
C -4.3577805 1.2894657 0.3935170

C	-5.0382829	-0.8941384	-0.3903361
H	-1.3241132	1.3832421	0.0838224
C	-0.3837748	-0.6408035	-0.0027686
C	-5.6886746	1.6987376	0.4038954
H	-3.5787027	1.9788574	0.7052201
C	-6.3696549	-0.4832398	-0.3724678
H	-4.8019010	-1.9001261	-0.7262610
C	1.0470602	-0.3707508	0.0180866
N	1.5058943	0.9171332	0.1015999
C	-6.7017695	0.8142117	0.0236694
H	-5.9364557	2.7095303	0.7152032
H	-7.1482248	-1.1770485	-0.6763715
N	1.9934991	-1.3463792	-0.0415168
C	2.8522926	0.7503320	0.0938511
H	-7.7397356	1.1335928	0.0347141
H	6.3893186	-0.2656059	-0.0146924
C	3.1478205	-0.6242676	0.0063809
C	3.9104870	1.7028159	0.1455431
C	4.4936685	-1.0393214	-0.0271089
N	5.1764560	1.3081637	0.0924909
N	5.4008819	-0.0420604	0.0135038
N	-2.2115145	-1.7316263	-0.0803296
N	-0.8725386	-1.8970491	-0.0717338
H	-2.8014288	-2.5533889	-0.0857117
N	3.6489765	3.0422172	0.3027760
H	4.3919170	3.6807781	0.0416008
H	2.7237008	3.3331657	0.0090582
N	4.8902272	-2.3346695	-0.0442506
H	5.8352096	-2.5721919	-0.3196229
H	4.1795497	-3.0129537	-0.2898234

2^{+}

35

Energy = -979.8012678726

C	2.6121374	-0.3783326	0.0297676
C	4.0316112	-0.0302493	0.0263823
C	1.4680207	0.4137840	-0.0043880
C	4.4328274	1.2549360	-0.3769246
C	5.0136251	-0.9540694	0.4232683
H	1.4140853	1.4909219	-0.0268672
C	0.3914313	-0.4963823	0.0262319
C	5.7803809	1.6047995	-0.3833139
H	3.6865463	1.9757471	-0.6973890
C	6.3614695	-0.6016732	0.4094144
H	4.7309959	-1.9460563	0.7648027
C	-1.0252429	-0.2206652	0.0157469
N	-1.5899961	0.9887109	-0.0464697
C	6.7504664	0.6778819	0.0071537
H	6.0744607	2.6013380	-0.6993543
H	7.1078878	-1.3262450	0.7211827
N	-1.9640299	-1.2248946	0.0683354
C	-2.9356208	0.7447345	-0.0341606
H	7.8013848	0.9512526	-0.0007472
H	-1.7458794	-2.2141810	0.1171050
C	-3.1943970	-0.6224627	0.0374973
C	-4.0267843	1.6678666	-0.0784673

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C    -4.5194053   -1.1093596    0.0660034
N    -5.2732356    1.2179436   -0.0385235
N    -5.4493707   -0.1333116    0.0211284
N     2.1562597   -1.6687037    0.0770342
N     0.8193127   -1.7759380    0.0723288
H    -6.4310096   -0.3911957    0.0380602
H     2.7121193   -2.5151769    0.0725126
N    -3.8024354    3.0015990   -0.2095757
H    -2.8795079    3.3389551    0.0327583
H    -4.5709216    3.6342126   -0.0233307
N    -4.8797055   -2.3983516    0.1408858
H    -4.1869079   -3.1323192    0.1357384
H    -5.8508489   -2.6805683    0.1379451
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3

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37
Energy = -1055.797700411
C     2.1901863    0.0686037    0.2714852
C     3.6453144    0.0748801    0.1635673
C     1.2462545   -0.0562820   -0.9026367
C     4.2590049   -0.0941052   -1.0900652
C     4.4617731    0.2419686    1.2998561
H     1.3088088    0.8119782   -1.5680713
H     1.4333212   -0.9559142   -1.4935740
C    -0.1309091   -0.1189966   -0.2231157
C     5.6491262   -0.0994175   -1.2059992
H     3.6484900   -0.2223300   -1.9791560
C     5.8462974    0.2336828    1.1796134
H     3.9947848    0.3779954    2.2703197
C    -0.7019852   -1.5476393   -0.2054366
N    -1.0959232    0.7857186   -0.8374705
C     6.4478571    0.0631562   -0.0736632
H     6.1064716   -0.2308867   -2.1824708
H     6.4637428    0.3627947    2.0642046
O     0.0120647   -2.5411237   -0.3229427
N    -2.0455083   -1.6270046    0.0480733
C    -2.4190004    0.6839913   -0.4478472
H     7.5303492    0.0594171   -0.1631512
H    -2.4418833   -2.5596936    0.1296750
C    -2.9043502   -0.5243569    0.0172251
C    -3.3518208    1.7452005   -0.5687678
C    -4.2522008   -0.5950230    0.4300113
N    -4.6235323    1.6117549   -0.2019434
N    -5.0693281    0.4547780    0.3346390
N     1.5733564    0.1961892    1.4046822
N     0.2047335    0.2800400    1.1814187
H    -0.7471904    1.7370760   -0.9276120
H    -0.3203361   -0.1710341    1.9280647
N    -2.9239182    2.9938799   -1.0235533
H    -3.7073450    3.6309189   -1.1493825
H    -2.3643264    2.9622150   -1.8728164
N    -4.7900981   -1.8014524    0.8773348
H    -4.2224832   -2.2926891    1.5635511
H    -5.7372497   -1.6799201    1.2280153
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A_ts

31
Energy = -943.7481849736
C 1.7495432 0.3680267 0.2602462
C 3.1963304 0.1806312 0.0479855
C 0.7386193 0.1532902 -0.8461294
C 4.0987447 0.3551569 1.1238057
C 3.7024146 -0.1656373 -1.2237170
H 0.7638000 1.0092242 -1.5426424
H 0.9806886 -0.7604605 -1.4120046
C -0.6668098 0.0482848 -0.2765720
C 5.4707807 0.1808580 0.9293025
H 3.7023463 0.6246790 2.1067450
C 5.0802416 -0.3354364 -1.4151318
H 3.0246832 -0.2990672 -2.0717356
C -0.9902480 -1.3119784 0.2930087
N -1.6240224 0.8057074 -0.8649432
C 5.9661090 -0.1646278 -0.3412442
H 6.1607577 0.3139451 1.7688682
H 5.4609635 -0.6018455 -2.4061402
O -0.1238976 -2.1342067 0.6004114
N -2.3348743 -1.5471442 0.4627919
C -2.9203576 0.5000694 -0.6025180
H 7.0423107 -0.2996106 -0.4914454
H -2.5972650 -2.4390921 0.8875094
C -3.3326117 -0.6495438 0.0791580
C -3.9139031 1.4180937 -1.0944661
C -4.6843337 -0.9675037 0.3546298
N -4.7087033 2.1764563 -1.4989159
N -5.8057433 -1.2308259 0.5854740
N 1.3170579 0.7618723 1.4178770
N -0.0952271 0.8947662 1.3845308
H -0.3604568 1.8889387 1.3064208
H -0.4944295 0.5393132 2.2648425

At
31
Energy = -943.7569816917
C 1.4510306 0.2413943 0.3315740
C 2.9078042 0.1750954 0.0824408
C 0.5688873 0.8508978 -0.7514151
C 3.5551669 1.2519220 -0.5501738
C 3.6676407 -0.9581052 0.4246328
H 0.5925108 1.9448589 -0.7211657
H 0.9340320 0.5260750 -1.7330302
C -0.8405780 0.3902123 -0.5775065
C 4.9234092 1.2090758 -0.8075681
H 2.9849786 2.1324658 -0.8324700
C 5.0352500 -1.0028830 0.1549475
H 3.1815181 -1.8185591 0.8731083
C -1.1091789 -1.0373371 -0.8553091
N -1.7643540 1.2367801 -0.2034904
C 5.6693521 0.0815642 -0.4539710
H 5.4077779 2.0547831 -1.2873724
H 5.6043058 -1.8904268 0.4167012
O -0.2887574 -1.8491895 -1.2697770
N -2.4352641 -1.4073408 -0.6193341

C	-3.0477685	0.7896257	-0.0162991
H	6.7356311	0.0466111	-0.6579033
H	-2.6762630	-2.3825647	-0.7841847
C	-3.3984160	-0.5341744	-0.2097027
C	-4.0232296	1.7451634	0.3924951
C	-4.7197450	-1.0199856	-0.0113486
N	-4.8162023	2.5269353	0.7252568
N	-5.8016156	-1.4102592	0.1513354
N	0.8158708	-0.1525235	1.3877477
N	1.4806826	-0.7480073	2.4306497
H	2.4690164	-0.4975095	2.5236803
H	0.9726945	-0.5790414	3.2932542

At^+

32

Energy = -944.1974704387

C	0.6737215	0.1343540	-0.8774983
C	2.0760968	0.5304052	-1.0386896
C	-0.1883275	0.9205212	0.0725631
C	3.1009273	-0.4343167	-1.0851668
C	2.4097299	1.8961986	-1.0916187
H	0.3131180	0.9393313	1.0505548
H	-0.1820796	1.9736917	-0.2421671
C	-1.6172584	0.5331890	0.3025684
C	4.4295744	-0.0337587	-1.1917625
H	2.8663282	-1.4895303	-0.9918176
C	3.7387142	2.2852636	-1.2199845
H	1.6322564	2.6522201	-1.0612214
C	-2.3413979	1.3865724	1.2664659
N	-2.1726297	-0.4838520	-0.2986534
C	4.7503745	1.3229687	-1.2691231
H	5.2140249	-0.7834610	-1.2106304
H	3.9848761	3.3405543	-1.2788687
O	-1.8584188	2.3501019	1.8463767
N	-3.6645581	0.9876293	1.4673100
C	-3.4814060	-0.8091516	-0.0536365
H	5.7872868	1.6306115	-1.3623443
H	-4.2127858	1.5379188	2.1270664
C	-4.2393426	-0.0716346	0.8378555
C	-4.0247906	-1.9253734	-0.7478950
C	-5.5990263	-0.3786617	1.1219037
N	-4.4586339	-2.8376223	-1.3215101
N	-6.7079617	-0.6352244	1.3486362
N	0.1472791	-0.8744723	-1.5087714
H	-0.8488043	-1.0838870	-1.2696895
N	0.7634525	-1.7548754	-2.3694686
H	0.0870246	-2.0581812	-3.0688613
H	1.5712613	-1.3211810	-2.8191790

A

31

Energy = -943.7612452069

C	1.5645042	1.1751668	0.1761462
C	2.7638027	0.3150974	0.2168321
C	0.6337721	1.1565455	-1.0432679
C	3.7491517	0.5155697	1.2055256

C	2.9616277	-0.7150302	-0.7180271
H	0.3176029	2.1929002	-1.2197603
H	1.1663347	0.7946558	-1.9223796
C	-0.5893424	0.3225648	-0.8200624
C	4.8876204	-0.2803153	1.2478931
H	3.6072817	1.3089381	1.9317459
C	4.1048214	-1.5153586	-0.6686638
H	2.2157675	-0.9124758	-1.4813100
C	-0.7040866	-0.9760997	-1.5153961
N	-1.5226104	0.7758089	-0.0155794
C	5.0746199	-1.3029163	0.3099062
H	5.6372564	-0.1027310	2.0144080
H	4.2330847	-2.3080468	-1.4007545
O	0.1140473	-1.4409667	-2.3042284
N	-1.8795020	-1.6661977	-1.2127924
C	-2.6425449	0.0326793	0.2316663
H	5.9653832	-1.9235965	0.3452579
H	-2.0109733	-2.5639738	-1.6751114
C	-2.8392233	-1.1999758	-0.3655820
C	-3.6092524	0.5742764	1.1278156
C	-3.9945801	-1.9949858	-0.1370262
N	-4.3933400	1.0188228	1.8609405
N	-4.9412794	-2.6398527	0.0553492
N	1.3717085	1.9912794	1.1628221
N	0.2905312	2.8293717	1.1445789
H	-0.5808885	2.4194302	0.7923640
H	0.1773641	3.2706306	2.0508399

Bn1

37

Energy = -1055.766244483

C	2.2441293	0.1073000	0.2592076
C	3.6964562	0.1125686	0.1194919
C	1.2761786	-0.1314080	-0.8770895
C	4.2847896	-0.1469615	-1.1309056
C	4.5362596	0.3691416	1.2217358
H	1.3190767	0.6708989	-1.6219863
H	1.4583095	-1.0820200	-1.3839628
C	-0.0876559	-0.1353695	-0.1659706
C	5.6721615	-0.1520201	-1.2767949
H	3.6562280	-0.3449272	-1.9942452
C	5.9178944	0.3601525	1.0721178
H	4.0891538	0.5741298	2.1894729
C	-0.6477827	-1.5619592	0.0074087
N	-1.0678807	0.7046142	-0.8313804
C	6.4939468	0.1000980	-0.1778436
H	6.1093460	-0.3532712	-2.2506551
H	6.5531137	0.5583310	1.9310234
O	0.0918171	-2.5455676	0.0484417
N	-1.9971823	-1.6375526	0.2048992
C	-2.3843560	0.6064832	-0.4593497
H	7.5742840	0.0963879	-0.2906017
H	-2.4162475	-2.5276700	0.4712856
C	-2.8652656	-0.5621959	0.0452141
C	-3.2625124	1.7506220	-0.6748477
C	-4.2555346	-0.7527171	0.3961627

N	-2.7762775	2.8211542	-1.2207973
N	-4.6361448	-1.8756685	0.9255847
N	1.6510187	0.3363940	1.3891831
N	0.2786558	0.3934745	1.1898486
H	-0.7757676	1.6507578	-1.0721781
H	-0.2286621	0.0112423	1.9858167
N	-5.0948698	0.2974986	0.0477212
H	-5.9257218	0.3843825	0.6269093
H	-5.6418055	-1.8847964	1.1167196
N	-4.5534391	1.5958481	-0.2035641
H	-5.2524357	2.1796795	-0.6543107
H	-3.4872056	3.5491459	-1.3355042

Bn2

37

Energy = -1055.788025879

C	2.2259834	0.2051923	0.1671385
C	3.6747435	0.2136378	-0.0050372
C	1.2317796	-0.0384162	-0.9456524
C	4.2360170	-0.0408628	-1.2687839
C	4.5379456	0.4659012	1.0800042
H	1.2394181	0.7760606	-1.6787766
H	1.4157447	-0.9778268	-1.4717081
C	-0.1106255	-0.0739344	-0.1961810
C	5.6199783	-0.0452486	-1.4443351
H	3.5890967	-0.2354637	-2.1192330
C	5.9160254	0.4574899	0.9008644
H	4.1117035	0.6662228	2.0580845
C	-0.6166876	-1.5121088	0.0158477
N	-1.1397976	0.7203453	-0.8383789
C	6.4651120	0.2022339	-0.3621699
H	6.0362490	-0.2427226	-2.4280835
H	6.5695091	0.6517495	1.7468705
O	0.1532672	-2.4715635	0.0500455
N	-1.9579042	-1.6363614	0.2655266
C	-2.4376363	0.5841708	-0.4217645
H	7.5428135	0.1982473	-0.4978528
H	-2.2733331	-2.5510596	0.5728717
C	-2.8796892	-0.5921889	0.1228363
C	-3.3420964	1.7049251	-0.5806946
C	-4.2540561	-0.7252530	0.5014143
N	-2.9059584	2.8217396	-1.0959494
N	-4.6977636	-1.9085148	1.1000587
N	1.6584199	0.4361882	1.3097506
N	0.2810976	0.4826461	1.1418968
H	-0.8935778	1.6781793	-1.0882802
H	-0.2042221	0.1087091	1.9554280
N	-5.1085948	0.2624303	0.3697970
H	-5.7009185	-1.8826320	1.2689032
H	-4.4681230	-2.7514767	0.5775447
N	-4.6152627	1.4383874	-0.1251002
H	-5.3141322	2.1696655	-0.1832130
H	-3.6474763	3.5254764	-1.1477820

Bn

37

Energy = -1055.742368270

C	-2.3497073	-0.1642257	0.2038243
C	-3.8079192	-0.1464677	0.1526719
C	-1.4513127	0.3102306	-0.9158067
C	-4.4664021	0.3677057	-0.9781297
C	-4.5824960	-0.6325028	1.2247752
H	-1.5674754	-0.2956749	-1.8209358
H	-1.6367135	1.3552279	-1.1778101
C	-0.0464685	0.1376258	-0.3170819
C	-5.8597862	0.3985226	-1.0361845
H	-3.8886310	0.7450775	-1.8168547
C	-5.9704434	-0.5972426	1.1633148
H	-4.0806133	-1.0350125	2.0991360
C	0.6156885	1.4744178	0.0413132
N	0.8463616	-0.5782132	-1.2175206
C	-6.6168953	-0.0820920	0.0326668
H	-6.3522469	0.7980930	-1.9181031
H	-6.5554696	-0.9744516	1.9975027
O	-0.0288073	2.4968611	0.2657451
N	1.9753772	1.4091932	0.1758253
C	2.1899701	-0.6969140	-0.8515338
H	-7.7019224	-0.0593299	-0.0122402
H	2.4903601	2.2063993	0.5590742
C	2.7724655	0.3146350	-0.1371142
C	2.8722045	-1.8443613	-1.3227615
C	4.1761601	0.4670898	0.3083849
N	3.3697644	-2.8105590	-1.7427369
N	4.5279236	1.6566797	0.6798790
N	-1.6916647	-0.6119573	1.2269795
N	-0.3327720	-0.6222887	0.9385503
H	0.4376594	-1.4063262	-1.6396676
H	0.2226113	-0.3897937	1.7595127
N	4.9816656	-0.6426905	0.2520370
H	4.5621388	-1.5630568	0.2706691
H	5.5029515	1.6820892	0.9895058
N	6.3070105	-0.6281472	0.7347373
H	6.8743613	-0.0439744	0.1197109
H	6.3335018	-0.2187709	1.6727743

B

31

Energy = -943.7691182750

C	1.7012932	0.1803476	0.2249963
C	3.1528618	0.1502157	0.0820901
C	0.7287709	-0.2061838	-0.8671086
C	3.7325221	-0.2735929	-1.1264751
C	3.9978961	0.5330036	1.1425826
H	0.7779266	0.4826455	-1.7176605
H	0.8983278	-1.2198842	-1.2370706
C	-0.6293450	-0.0986744	-0.1547248
C	5.1190925	-0.3153459	-1.2723831
H	3.0992878	-0.5709719	-1.9572250
C	5.3787231	0.4863711	0.9932997
H	3.5565524	0.8636843	2.0775535
C	-1.2200549	-1.4747225	0.1851779
N	-1.6019244	0.6589411	-0.9365325

C	5.9467594	0.0626928	-0.2147585
H	5.5508815	-0.6438036	-2.2133567
H	6.0192924	0.7819932	1.8194281
O	-0.5224921	-2.4731596	0.3256475
N	-2.5755963	-1.4886267	0.4122979
C	-2.9205492	0.6610853	-0.5501367
H	7.0265541	0.0296697	-0.3273897
H	-2.9753918	-2.3546837	0.7630786
C	-3.4259991	-0.4135437	0.1395332
C	-3.7443622	1.7590248	-0.9081549
C	-4.7678430	-0.4864212	0.5662848
N	-4.4017239	2.6649547	-1.2233094
N	-5.8747119	-0.5719712	0.9189296
N	1.1122530	0.5669113	1.3125170
N	-0.2626415	0.6007471	1.1091753
H	-1.2507249	1.5012724	-1.3805083
H	-0.7713233	0.3370880	1.9508936

B^+

32

Energy = -944.1930815214

C	1.7307400	-0.1502010	0.3615622
C	3.1295871	0.1203346	0.0537976
C	0.7121990	-0.5379920	-0.6821726
C	4.0371852	0.4412298	1.0824028
C	3.5821286	0.0477320	-1.2748128
H	0.7353513	0.1036127	-1.5646979
H	0.8825665	-1.5702967	-1.0027812
C	-0.6370969	-0.4310249	0.0297964
C	5.3691667	0.6868673	0.7790435
H	3.6875039	0.4922908	2.1080921
C	4.9203633	0.2932582	-1.5706643
H	2.8960529	-0.2028026	-2.0773429
C	-1.5199439	-1.6805938	-0.1128485
N	-1.3118619	0.7807807	-0.2435743
C	5.8134254	0.6133629	-0.5467997
H	6.0667104	0.9339879	1.5731351
H	5.2646506	0.2344063	-2.5981558
O	-1.0093027	-2.7916921	-0.1076382
N	-2.8624544	-1.4643984	-0.1970436
C	-2.6851469	0.9078393	-0.1898642
H	6.8567901	0.8048742	-0.7785975
H	-3.4516044	-2.2926489	-0.2459968
C	-3.4716633	-0.2098690	-0.1577495
C	-3.2397171	2.2118805	-0.2064702
C	-4.8813408	-0.1487779	-0.0900113
N	-3.6763941	3.2883372	-0.2319994
N	-6.0429691	-0.1159406	-0.0454171
N	1.2895946	-0.0912387	1.5791622
N	-0.1125709	-0.4590926	1.5549534
H	-0.6431071	0.1934449	2.1444645
H	-0.2066623	-1.3999882	1.9617826
H	-0.7620438	1.6072133	-0.4501046

C^+

38

Energy = -1056.208782375

C	2.1442746	-0.0824920	0.2739433
C	3.5901099	0.0883612	0.1882552
C	1.2815315	-0.5843819	-0.8668131
C	4.2703536	-0.2728793	-0.9870653
C	4.3241872	0.6007037	1.2752860
H	1.3737136	0.0138728	-1.7769640
H	1.5155400	-1.6226011	-1.1218262
C	-0.1169715	-0.5059049	-0.2566195
C	5.6546143	-0.1318245	-1.0729482
H	3.7211654	-0.6680465	-1.8366287
C	5.7038963	0.7378715	1.1841351
H	3.8011741	0.8869016	2.1821476
C	-0.8912705	-1.8354732	-0.2748216
N	-0.9667886	0.5816999	-0.9975706
C	6.3746294	0.3723381	0.0107152
H	6.1686974	-0.4157593	-1.9862516
H	6.2622461	1.1330993	2.0276244
O	-0.3082000	-2.9033370	-0.3549873
N	-2.2471982	-1.7255141	-0.0900374
C	-2.3434041	0.6427710	-0.5033613
H	7.4528330	0.4835431	-0.0562945
H	-2.7706162	-2.5959296	-0.0312697
C	-2.9277318	-0.5142799	-0.0508147
C	-3.0305889	1.8640058	-0.4429753
C	-4.2412970	-0.3893215	0.4819963
N	-4.2581716	1.9159625	0.0837554
N	-4.8388033	0.8045169	0.5549707
N	1.4673032	0.1516976	1.3514069
N	0.1004253	-0.0081226	1.0859832
H	-0.9368433	0.4133044	-2.0123865
H	-0.3953693	-0.4494537	1.8555262
N	-2.4081172	3.0401472	-0.8341018
H	-2.9979891	3.8542594	-0.6769774
H	-2.0497711	3.0487864	-1.7857565
N	-4.9546238	-1.4981266	0.8781164
H	-4.4454233	-2.2206582	1.3768727
H	-5.8301229	-1.2682655	1.3399290
H	-0.5202831	1.4963536	-0.8210189

Dc

37

Energy = -1055.783188478

C	2.0843779	-0.0057724	-0.6255130
C	3.4681749	0.1674997	-0.1974404
C	1.3662550	-1.3146399	-0.7791353
C	4.2846681	-0.9523276	0.0380629
C	4.0038756	1.4567744	-0.0125425
H	1.8067230	-1.9622423	-1.5468084
H	1.3250413	-1.8967169	0.1488083
C	0.0307808	-0.7913186	-1.1851007
C	5.6065979	-0.7884131	0.4461426
H	3.8860990	-1.9529965	-0.1010123
C	5.3231334	1.6152229	0.3954069
H	3.3713779	2.3204327	-0.1900806
C	-1.1289021	-1.6365177	-1.5750601

N	-3.7869555	1.1979961	-1.8616545
C	6.1290115	0.4942313	0.6256215
H	6.2284734	-1.6607012	0.6237802
H	5.7277856	2.6130625	0.5373962
O	-0.9567869	-2.6747367	-2.2229196
N	-2.3728581	-1.1990370	-1.2086400
C	-3.3294771	0.9564770	-0.5909610
H	7.1593539	0.6218818	0.9446703
H	-3.1414585	-1.7819003	-1.5345058
C	-2.6494438	-0.1953885	-0.2346659
C	-3.5651357	1.8968835	0.4583428
C	-2.2166976	-0.3374867	1.1031710
N	-3.1211330	1.7145291	1.6922653
N	-2.4312260	0.6006369	2.0282228
N	1.3039351	1.0017248	-0.9211908
N	0.0143538	0.5028913	-1.2737289
H	-3.3602187	0.6397306	-2.5942539
N	-4.2050194	3.1021412	0.1533784
H	-4.3813608	3.6520261	0.9910366
H	-5.0653710	2.9904247	-0.3794075
N	-1.4595521	-1.4387373	1.4820464
H	-1.7351894	-2.3180652	1.0561575
H	-1.3640291	-1.5202558	2.4898104
H	-3.8850800	2.1758747	-2.1149746

Dc^{+}

38

Energy = -1056.223181928

C	2.1280871	-0.4521329	0.1745001
C	3.4926061	0.0260133	0.1368828
C	1.3462497	-1.0024123	-0.9904295
C	4.2289272	-0.0381890	-1.0611476
C	4.0929378	0.5591019	1.2967107
H	1.2563768	-0.2963766	-1.8253385
H	1.7753593	-1.9218188	-1.4084910
C	0.0414273	-1.2727764	-0.3380344
C	5.5406783	0.4208614	-1.0984071
H	3.7775376	-0.4478534	-1.9595505
C	5.4029233	1.0150392	1.2505701
H	3.5228348	0.6095696	2.2182616
C	-1.1320609	-2.0054986	-0.9131501
N	-3.1610552	0.7106925	-2.2559963
C	6.1286537	0.9472445	0.0552517
H	6.1052798	0.3689933	-2.0236992
H	5.8636581	1.4254448	2.1435054
O	-0.8971027	-3.0260000	-1.5549999
N	-2.3809136	-1.5258822	-0.6572766
C	-3.0898555	0.7973251	-0.9030358
H	7.1531311	1.3056312	0.0242141
H	-3.1336236	-2.0939361	-1.0444673
C	-2.7190872	-0.2610395	-0.0779107
C	-3.4384112	2.0176260	-0.2313771
C	-2.7108246	-0.0489846	1.3152755
N	-3.3804082	2.1493912	1.0865381
N	-3.0003792	1.1188953	1.8739834
N	1.4052199	-0.4414953	1.2762119

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N     0.1625845   -0.9465868    0.9147951
H    -2.7902330   -0.1107230   -2.7167194
H    -0.6251191   -1.0517396    1.6418248
N    -3.7698966    3.1287236   -0.9898195
H    -4.0826799    3.9113240   -0.4212438
H    -4.4118489    2.9556974   -1.7591472
N    -2.2316891   -1.0597771    2.1800110
H    -2.6294819   -1.9796596    1.9930558
H    -2.3905991   -0.8068279    3.1544520
H    -3.1101986    1.5635838   -2.7992532
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D

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37
Energy = -1055.791463292
C    -2.9452175    0.1598595   -0.0638723
C    -4.3919279    0.0011510   -0.0065066
C    -1.9275273   -0.8417073    0.3993595
C    -4.9555899   -1.1787932    0.5108680
C    -5.2442085    1.0241588   -0.4667968
H    -2.0037998   -1.0720156    1.4688668
H    -1.9894356   -1.7989936   -0.1322434
C    -0.6926221   -0.0819431    0.0647996
C    -6.3383904   -1.3342241    0.5655381
H    -4.3115020   -1.9761351    0.8696265
C    -6.6234408    0.8640848   -0.4094554
H    -4.8092146    1.9350101   -0.8649175
C     0.6965503   -0.5348227    0.3071283
N     3.3004987   -2.0754782   -0.5786563
C    -7.1750479   -0.3144747    0.1061238
H    -6.7630516   -2.2497538    0.9660537
H    -7.2739452    1.6572192   -0.7659997
O     0.9358790   -1.6283886    0.8455134
N     1.6389692    0.3601598   -0.0984385
C     3.8099093   -0.8456252   -0.2419575
H    -8.2534856   -0.4359530    0.1489033
H     1.2616420    1.2344236   -0.4687836
C     3.0429708    0.2912457    0.0014586
C     5.2276078   -0.6435368   -0.2310546
C     3.7221885    1.5005278    0.3022102
N     5.7999613    0.5226601    0.0245029
N     5.0483800    1.6039235    0.3359321
N    -2.3682242    1.2360192   -0.5454987
N    -0.9628479    1.0752486   -0.4611952
H     2.3681230   -2.2581560   -0.1965031
N     6.0610589   -1.7446276   -0.4545442
H     7.0364074   -1.4597619   -0.5099368
H     5.8151892   -2.2920106   -1.2770644
N     2.9836694    2.6664080    0.5035395
H     2.1882011    2.5636448    1.1284055
H     3.5751678    3.4384880    0.8004586
H     3.9405083   -2.8487372   -0.4219939
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D^+

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38
Energy = -1056.229867241
C    -2.9936395    0.1698498   -0.0856972
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C	-4.4156987	0.0091965	-0.0260924
C	-1.9281213	-0.7796711	0.3589991
C	-4.9421287	-1.1878335	0.5054168
C	-5.2935466	1.0174619	-0.4840937
H	-1.9922100	-1.0090537	1.4297867
H	-1.9769397	-1.7410297	-0.1672711
C	-0.6993387	-0.0050112	0.0146732
C	-6.3157801	-1.3705514	0.5758236
H	-4.2740012	-1.9664690	0.8583445
C	-6.6635764	0.8247049	-0.4085972
H	-4.9104514	1.9463056	-0.8951073
C	0.6861240	-0.4706417	0.2732834
N	3.2691960	-2.0727527	-0.5574716
C	-7.1761879	-0.3669194	0.1200497
H	-6.7184618	-2.2913311	0.9839899
H	-7.3375373	1.5988321	-0.7595153
O	0.8771018	-1.5711451	0.8110170
N	1.6469205	0.4071378	-0.1091528
C	3.7928985	-0.8524773	-0.2263646
H	-8.2505961	-0.5114496	0.1760661
H	1.3162907	1.3014266	-0.4748153
C	3.0480744	0.3028737	0.0052709
C	5.2158037	-0.6720083	-0.2123139
C	3.7451463	1.5042105	0.2980540
N	5.8040889	0.4890923	0.0283747
N	5.0708620	1.5855926	0.3306912
N	-2.3542827	1.2261461	-0.5620540
N	-0.9681339	1.1484602	-0.5164379
H	2.3245248	-2.2467344	-0.2067652
H	-2.7597645	2.0717478	-0.9538698
N	6.0306757	-1.7865609	-0.4185427
H	7.0120963	-1.5226583	-0.4678230
H	5.7808739	-2.3467650	-1.2308762
N	3.0186964	2.6808104	0.4880669
H	2.2591863	2.6055399	1.1604767
H	3.6279704	3.4584731	0.7308460
H	3.8942113	-2.8588516	-0.4061313

Ec$^+$

38

Energy = -1056.217234687

C	-2.5008148	-0.2679337	-0.0574653
C	-3.9294945	0.0139168	-0.1796831
C	-1.6217296	-0.1133064	1.0173996
C	-4.7084607	0.1704603	0.9792789
C	-4.5460877	0.1335696	-1.4366719
H	-1.8498220	0.2736617	1.9981687
H	1.5893563	-0.8828476	2.9941243
C	-0.3839753	-0.5585127	0.5320909
C	-6.0711753	0.4379370	0.8814993
H	-4.2473834	0.0680935	1.9570211
C	-5.9109703	0.3959558	-1.5292971
H	-3.9615759	0.0436808	-2.3481483
C	0.9548477	-0.6003958	1.1985154
N	1.8898618	-1.4527384	0.2156659
C	-6.6779730	0.5493003	-0.3721933

```
H    -6.6616417    0.5536688    1.7854608
H    -6.3738642    0.4882936   -2.5071423
O     0.8682135   -1.2146048    2.4245982
N     1.6760091    0.6701115    1.2631508
C     2.9853305   -0.5629641   -0.1617868
H    -7.7413893    0.7558950   -0.4468317
H     1.0956736    1.5042680    1.2944756
C     2.7826958    0.6565291    0.4288987
C     4.0923086   -0.7990575   -0.9857365
C     3.7300505    1.6758879    0.1772346
N     4.9478152    0.2154443   -1.2020426
N     4.7692420    1.4123754   -0.6195366
N    -1.7483474   -0.7785665   -1.0764553
N    -0.4602409   -0.9648585   -0.7441670
H     1.2673430   -1.7087004   -0.5843847
H    -2.0637291   -1.0658478   -1.9949073
N     4.3923363   -2.0262586   -1.5305376
H     3.6162644   -2.6292092   -1.7789040
H     5.1041391   -1.9900837   -2.2541668
N     3.5673074    2.9554409    0.6729185
H     3.1892319    3.0179872    1.6133515
H     4.3902818    3.5400516    0.5562808
H     2.1878549   -2.2999002    0.7118298
```

E

```
37
Energy = -1055.825086841
C    -2.9321589    0.1134575   -0.0548461
C    -4.3865353   -0.0096229    0.0200813
C    -1.9088802   -0.7028571    0.4203922
C    -4.9670887   -1.2572503    0.3064744
C    -5.2275293    1.0980529   -0.1835080
H    -2.0056752   -1.6228703    0.9754973
C    -0.7158582   -0.0537281    0.0488603
C    -6.3506486   -1.3917386    0.3859369
H    -4.3305838   -2.1245425    0.4543719
C    -6.6117830    0.9576972   -0.1093935
H    -4.8058879    2.0800944   -0.3796409
C     0.6693891   -0.4789815    0.3302830
N     3.2769322   -2.0890327   -0.4358506
C    -7.1791579   -0.2861227    0.1761138
H    -6.7833918   -2.3632064    0.6063027
H    -7.2473022    1.8241800   -0.2668989
O     0.9235082   -1.5190416    0.9604017
N     1.6185130    0.3754934   -0.1520627
C     3.7894898   -0.8386340   -0.1830285
H    -8.2582039   -0.3928230    0.2363336
H     1.2506304    1.2160842   -0.5983509
C     3.0225199    0.3130548   -0.0302879
C     5.2069686   -0.6408344   -0.1671729
C     3.7025008    1.5377063    0.1933159
N     5.7812509    0.5384777    0.0150232
N     5.0290264    1.6409790    0.2371206
N    -2.2999990    1.1664922   -0.6614815
N    -0.9621076    1.0913464   -0.6190287
H     2.3436799   -2.2356831   -0.0394066
```

```
H    -2.7307748    1.9382433   -1.1560130
N     6.0398071   -1.7576363   -0.3023855
H     7.0163457   -1.4789437   -0.3677590
H     5.8011082   -2.3601015   -1.0876991
N     2.9667306    2.7184963    0.3022201
H     2.1542735    2.6557738    0.9103459
H     3.5554645    3.5032791    0.5698114
H     3.9122506   -2.8500346   -0.2134550
```

E^+

```
38
Energy = -1056.239728877
C    -2.4873408   -0.2511481    2.1680301
C    -3.7713357   -0.4369989    2.8384455
C    -1.2009325   -0.6600589    2.5046825
C    -3.9224536   -1.4711172    3.7773062
C    -4.8625134    0.4044986    2.5642141
H    -0.9132049   -1.2106526    3.3882607
H     1.3418655   -1.1707941    2.9336068
C    -0.3853716   -0.1736994    1.4604045
C    -5.1400109   -1.6586653    4.4254577
H    -3.0906565   -2.1370913    3.9864722
C    -6.0799503    0.2088661    3.2119389
H    -4.7615286    1.2287272    1.8636123
C     1.0390620   -0.2653347    1.2789665
N     3.5425432   -2.0362247    0.0953276
C    -6.2227859   -0.8215823    4.1437237
H    -5.2458664   -2.4634432    5.1465895
H    -6.9148886    0.8678169    2.9941569
O     1.8325738   -0.8535292    2.1508686
N     1.6071956    0.2532378    0.2072229
C     3.8577861   -0.7400981   -0.1739423
H    -7.1723500   -0.9707514    4.6487472
H     0.9577653    0.7329342   -0.4223190
C     2.9888857    0.3453596   -0.1188789
C     5.1757922   -0.4309301   -0.6568163
C     3.4619711    1.6284490   -0.4915738
N     5.5525351    0.7870088   -1.0071009
N     4.7116842    1.8397969   -0.8951251
N    -2.3501671    0.4279853    0.9830139
N    -1.1032538    0.4919422    0.5277344
H     2.7093778   -2.2425934    0.6297690
H    -3.0925396    0.8395144    0.4272400
N     6.1208851   -1.4548255   -0.7077310
H     6.9931554   -1.1340805   -1.1218857
H     5.8030624   -2.2997193   -1.1787016
N     2.5848260    2.7049909   -0.5096738
H     1.9879186    2.8005185    0.3066934
H     3.0569484    3.5807954   -0.7191962
H     4.3173802   -2.6558919    0.3051665
```

F

```
34
Energy = -979.3417261412
C     2.6006095   -0.3641317    0.0201292
C     4.0212186   -0.0202459    0.0210656
```

C	1.4586102	0.4315396	-0.0093345
C	4.4279844	1.2673429	-0.3694723
C	5.0011424	-0.9508070	0.4080173
H	1.4077100	1.5090316	-0.0227913
C	0.3766624	-0.4733548	0.0094239
C	5.7768449	1.6125910	-0.3731034
H	3.6839646	1.9937508	-0.6825187
C	6.3504037	-0.6033656	0.3967344
H	4.7150278	-1.9451993	0.7395538
C	-1.0411431	-0.1847042	-0.0059209
N	-1.5889757	1.0280026	-0.0460520
C	6.7443229	0.6786608	0.0072290
H	6.0740445	2.6113548	-0.6793869
H	7.0942464	-1.3341239	0.7004852
N	-1.9887516	-1.1845725	0.0133737
C	-2.9491224	0.7934077	-0.0539773
H	7.7962622	0.9483683	0.0014642
H	-1.7820652	-2.1761621	0.0259419
C	-3.2221758	-0.5741208	-0.0155349
C	-4.0469504	1.6875979	-0.1055658
C	-4.5581761	-1.0281382	-0.0168363
N	-5.2927371	1.2111278	-0.0964169
N	-5.5396481	-0.1285274	-0.0466077
N	2.1420982	-1.6527719	0.0546693
N	0.8013317	-1.7539222	0.0442181
H	2.6939611	-2.5011324	0.0403436
N	-3.8589507	3.0496702	-0.2284855
H	-4.6609070	3.6141694	0.0322985
H	-2.9808713	3.3986063	0.1393215
N	-4.8955696	-2.3774308	-0.0656261
H	-5.8808334	-2.5349320	0.1313343
H	-4.3094419	-2.9874259	0.4965061

F+

35

Energy = -979.7815669551

C	2.6473760	-0.3658704	0.1170025
C	4.0693857	-0.0366699	0.0554754
C	1.5109477	0.4219895	-0.0353892
C	4.4828673	1.2961199	0.2195337
C	5.0378620	-1.0296267	-0.1689624
H	1.4802868	1.4785264	-0.2543801
C	0.4299923	-0.4700022	0.1310507
C	5.8341329	1.6257883	0.1616075
H	3.7454045	2.0706888	0.4075652
C	6.3891516	-0.6952069	-0.2203869
H	4.7418986	-2.0630093	-0.3267917
C	-0.9807787	-0.2258163	0.0781010
N	-1.5948266	0.9503642	-0.1640405
C	6.7919457	0.6318991	-0.0560223
H	6.1406102	2.6591625	0.2930902
H	7.1270890	-1.4717974	-0.3973082
N	-1.9395036	-1.1548117	0.2696721
C	-2.9705491	0.7738070	-0.1248315
H	7.8457004	0.8903978	-0.0985014
H	-1.7293616	-2.1242901	0.4840444

```
C    -3.1886056   -0.5685101    0.1465294
C    -4.0714504    1.6423907   -0.2870458
C    -4.5108588   -1.0573505    0.2295700
N    -5.2973887    1.1237645   -0.1801242
N    -5.5105534   -0.1907227    0.0474982
N     2.1790537   -1.6318637    0.3565651
N     0.8485587   -1.7317729    0.3749874
H    -1.1053927    1.8157532   -0.3607763
H     2.7305677   -2.4600597    0.5504867
N    -3.9382655    2.9704371   -0.6264355
H    -3.1468123    3.4668856   -0.2316540
H    -4.8027904    3.4978628   -0.5449574
N    -4.8110256   -2.3581927    0.5645357
H    -4.1784894   -3.0766263    0.2296444
H    -5.7863072   -2.6018634    0.4183277
```

H_2O

```
3
Energy = -76.47556893053
O     0.0515808    0.0515816    0.0000000
H    -0.0667315    1.0151497    0.0000000
H     1.0151507   -0.0667312    0.0000000
```

H_2SO_4

```
7
Energy = -700.5108154583
S     0.0861900    0.1603805    0.1475427
O     0.1907360    1.0341245    1.2783607
O     0.2673856    0.6180440   -1.2080866
O    -1.3437205   -0.5308880    0.2862106
H    -1.6212814   -0.9126164   -0.5715430
O     1.1044278   -1.0293681    0.4458774
H     1.3162345   -1.5109675   -0.3797275
```

HSO_4^-

```
6
Energy = -700.0776746642
S     0.1080494    0.0220073   -0.0622012
O     0.1660468    0.6734083    1.2537977
O     0.3584534    0.9119027   -1.1972262
O    -1.4868844   -0.3544150   -0.3008805
H    -1.7582552   -0.9543001    0.4192867
O     0.8272899   -1.2580011   -0.1143436
```

$N_2H_4.OH_2$

```
9
Energy = -188.4190323618
N     0.8536851    0.9230824   -0.0086708
H     0.9400882    1.4822442   -0.8568318
H    -0.1229954    0.6098560    0.0379660
N     1.7184734   -0.2380418   -0.2059509
H     1.9117320   -0.6080994    0.7241627
H     1.2028650   -0.9734581   -0.6969832
O    -1.9029486   -0.5199041    0.1301214
H    -1.9619852   -0.8808021    1.0297315
H    -2.6492195    0.0992530    0.0755841
```

N_2H_4
6
Energy = -111.9377069434
N -0.1719944 0.7382799 0.0181870
H 0.2614902 -0.1887077 0.0207421
H 0.2644035 1.1969654 0.8221829
N 0.4537080 1.4187112 -1.1603870
H 0.0203364 0.9576119 -1.9646424
H 0.0174585 2.3444155 -1.1653677

$NH_2NH_3^+$
7
Energy = -112.3948611427
N -0.1495775 0.7320212 0.0294268
H 0.2350060 -0.2144289 0.0212158
H 0.2574999 1.2065075 0.8374261
N 0.4048067 1.3944815 -1.1392244
H 0.0481992 0.9318843 -1.9810615
H 0.0690635 2.3623257 -1.1604436
H 1.4318097 1.4063473 -1.1855516

SO_4^{2-}
5
Energy = -699.5889828396
S -0.0054365 -0.0009867 -0.0841437
O 0.1755806 0.6830801 1.2417000
O 0.4185967 0.9261209 -1.1883016
O -1.4515437 -0.3675911 -0.2655024
O 0.8357580 -1.2457210 -0.1246062

TS10$^+$
38
Energy = -1056.213096175
C -2.6853762 0.0610964 -0.2735404
C -4.1343746 -0.1151079 -0.2049396
C -1.7545490 0.4225363 0.6985635
C -4.7599229 -0.2445914 1.0468079
C -4.9240718 -0.1492972 -1.3668014
H -1.9454737 0.6645237 1.7321671
H 1.6073883 1.8769424 1.8870148
C -0.5213582 0.4460600 0.0224000
C -6.1401434 -0.4043445 1.1324683
H -4.1615338 -0.2312066 1.9527982
C -6.3042698 -0.3148586 -1.2763637
H -4.4714414 -0.0265147 -2.3468007
C 0.8125670 0.7769153 0.5265026
N 1.6997292 -0.8383711 0.9231474
C -6.9174671 -0.4420412 -0.0280683
H -6.6093495 -0.5042489 2.1066510
H -6.9017465 -0.3362706 -2.1827896
O 0.7976550 1.3494653 1.7495100
N 1.7438354 1.2826265 -0.4035906
C 3.0120622 -0.5063592 0.4320873
H -7.9938656 -0.5678203 0.0401103
H 1.3639247 1.3390904 -1.3508589

C	3.0034669	0.6556370	-0.3004533
C	4.2138297	-1.2223441	0.5858787
C	4.2114721	1.1063236	-0.8728121
N	5.3376452	-0.7364141	0.0331164
N	5.3334272	0.4024568	-0.6721640
N	-1.9595482	-0.1036433	-1.4233275
N	-0.6471973	0.1165661	-1.2770095
H	1.2857504	-1.6588847	0.4721271
H	-2.3056820	-0.3876558	-2.3322207
N	4.3120673	-2.3631038	1.3495233
H	3.4953091	-2.9615298	1.3947958
H	5.1724273	-2.8830549	1.2068728
N	4.2557770	2.2130339	-1.6907008
H	3.5911121	2.9500191	-1.4784076
H	5.1919016	2.5626314	-1.8704873
H	1.6322591	-0.9316516	1.9393892

TS11^{+}

38

Energy = -1056.172655296

C	2.6485417	-0.2749114	-0.0108996
C	4.0870378	-0.0448654	-0.1265624
C	1.6637330	0.3990675	0.7101920
C	4.6259984	1.1958586	0.2538863
C	4.9509205	-1.0436635	-0.6069681
H	1.7981420	1.2446893	1.3665517
H	-1.3674545	-0.0952081	2.9557999
C	0.4763023	-0.3007468	0.4324480
C	5.9947055	1.4303573	0.1551091
H	3.9689830	1.9809178	0.6159536
C	6.3190253	-0.8023746	-0.7096402
H	4.5648590	-2.0207929	-0.8836643
C	-0.9018695	-0.0534534	0.8888712
N	-1.6310088	1.2220421	0.4444881
C	6.8460664	0.4336716	-0.3288945
H	6.3968372	2.3945947	0.4513236
H	6.9747058	-1.5844798	-1.0803794
O	-0.8624410	0.4914749	2.3532251
N	-1.8217493	-1.0966950	0.7111667
C	-2.9053370	0.7703080	-0.0335115
H	7.9132159	0.6185304	-0.4072448
H	-1.4332189	-1.9812736	0.3887773
C	-3.0022928	-0.5862703	0.1485998
C	-3.9682742	1.4842100	-0.6050962
C	-4.1838894	-1.2425869	-0.2460320
N	-5.0692384	0.8082025	-0.9698444
N	-5.1686147	-0.5198403	-0.7950139
N	1.9961005	-1.2956006	-0.6459151
N	0.6777603	-1.3346193	-0.4036567
H	-1.1071862	1.8384572	-0.1814968
H	2.3917631	-1.9739251	-1.2858115
N	-3.8986893	2.8327719	-0.8890678
H	-3.4032694	3.4090567	-0.2167824
H	-4.7928156	3.2356963	-1.1545628
N	-4.3227860	-2.6154117	-0.1753004
H	-3.9092070	-3.0609126	0.6377310

H	-5.2733469	-2.9333319	-0.3421161
H	-1.4912309	1.3700276	1.7815841

TS1

37

Energy = -1096.695870102

C	1.3043567	-0.0351258	0.3296140
O	0.7578058	1.2133555	0.5164969
C	2.7061746	-0.0426865	-0.2665603
C	0.3264642	-0.9261922	-0.4851036
C	3.4474227	1.1425917	-0.3068516
C	3.2774189	-1.2192301	-0.7729617
H	0.6070881	-0.8925271	-1.5383626
H	0.3838910	-1.9705130	-0.1526199
C	-1.0865631	-0.4366706	-0.3839419
C	4.7425545	1.1495689	-0.8255271
H	2.9969883	2.0626543	0.0492222
C	4.5738379	-1.2138176	-1.2891561
H	2.7106635	-2.1463003	-0.7831719
C	-1.8001480	-0.5678743	0.8955607
N	-1.6446136	0.0676831	-1.4550822
C	5.3114756	-0.0289183	-1.3122037
H	5.3048464	2.0785239	-0.8550199
H	5.0020251	-2.1329388	-1.6782670
O	-1.3351481	-1.0562081	1.9321712
N	-3.1056655	-0.1020461	0.8661341
C	-2.9363731	0.5152660	-1.4001829
H	6.3191518	-0.0221308	-1.7175934
H	-3.6400691	-0.1782541	1.7301031
C	-3.6871922	0.4383240	-0.2410437
C	-3.4947695	1.0637022	-2.5924102
C	-5.0319878	0.8897785	-0.1538052
N	-3.9487630	1.5102687	-3.5638950
N	-6.1307483	1.2605921	-0.0939888
N	1.4190834	-0.6147995	1.8080418
H	1.2828163	1.6483294	1.4282233
H	0.4430402	-0.8154291	2.0939222
N	2.2085371	-1.7739969	2.1094375
H	1.8784774	-2.5478176	1.5285301
H	3.1652253	-1.5707642	1.8141129
O	1.8747324	1.7604317	2.6256008
H	1.7685887	0.2880650	2.3691450
H	2.7854716	2.0760537	2.5145684

TS2^{+}

41

Energy = -1132.613452246

C	1.2579800	-1.3120350	0.3546650
O	2.7581150	-1.4080000	1.6327130
C	1.9819160	-0.6121040	-0.7416470
C	0.4220080	-0.5310690	1.3428920
C	2.8437800	-1.3166250	-1.5974420
C	1.8339070	0.7700070	-0.9201790
H	0.1200550	-1.2326150	2.1265740
H	1.0198010	0.2549840	1.7944920
C	-0.8170760	0.0692750	0.7428020

C	3.5336770	-0.6525410	-2.6073670
H	3.0106000	-2.3817560	-1.4626790
C	2.5256280	1.4345340	-1.9333860
H	1.1853800	1.3438250	-0.2662880
C	-1.0178990	1.5169980	0.9470790
N	-1.6676840	-0.6899600	0.1037120
C	3.3773110	0.7252840	-2.7800460
H	4.2020050	-1.2111700	-3.2549420
H	2.3971560	2.5051810	-2.0573360
O	-0.2092220	2.2802540	1.4766800
N	-2.2349190	1.9800520	0.4545710
C	-2.8244550	-0.1466410	-0.3817980
H	3.9202550	1.2417010	-3.5652970
H	-2.4419120	2.9680390	0.5930540
C	-3.1332840	1.1908420	-0.1979290
C	-3.7168220	-1.0146190	-1.0771050
C	-4.3430800	1.7759190	-0.6616890
N	-4.4383570	-1.7260530	-1.6448650
N	-5.3333210	2.2439150	-1.0469220
N	0.8359020	-2.5473110	0.0702660
H	3.3492930	-2.0637540	1.2230860
H	1.2155300	-3.0287690	-0.7398160
N	0.0398880	-3.2804750	0.9765320
H	-0.8376780	-3.5049240	0.5064170
H	0.5185440	-4.1568510	1.1861520
N	3.1155700	1.9283000	2.2664410
H	2.2122430	1.9616330	1.7834910
H	2.9141400	1.5776450	3.2050920
N	3.8969930	0.8683670	1.6178120
H	4.0851110	1.1803950	0.6615840
H	4.8040460	0.8456440	2.0884520
H	3.3905580	-0.2324300	1.6094670

TS3

34

Energy = -1020.227066597

C	-1.7667227	0.0774191	-0.3722950
C	-3.0950833	-0.0673087	0.2269589
C	-0.4846219	-0.2620246	0.3450019
C	-4.2562942	0.2367847	-0.5078363
C	-3.2193898	-0.5186605	1.5507486
H	-0.3254371	0.3756125	1.2201085
H	-0.4747871	-1.3038003	0.6795099
C	0.5987739	0.0302323	-0.7260162
C	-5.5095077	0.0882723	0.0738531
H	-4.1613875	0.5864045	-1.5307491
C	-4.4789211	-0.6643200	2.1304850
H	-2.3328938	-0.7543850	2.1314247
C	1.2787208	-1.2563170	-1.2193235
N	1.5759003	1.0246922	-0.3036391
C	-5.6251210	-0.3622809	1.3944047
H	-6.4012937	0.3233085	-0.4996166
H	-4.5632437	-1.0128453	3.1553217
O	0.8865251	-1.8699159	-2.2160547
N	2.3275880	-1.6386905	-0.4489885
C	2.5939057	0.5607143	0.4394875

H	-6.6066316	-0.4760204	1.8452495
H	2.7752305	-2.5233212	-0.6703635
C	2.9438084	-0.7841019	0.4922348
C	3.3676495	1.5159899	1.1731638
C	3.9055619	-1.3159252	1.3615708
N	3.9935880	2.3049312	1.7529982
N	4.7163067	-1.7683714	2.0717161
N	-1.6114226	0.5133674	-1.5774275
N	-0.2092880	0.6106882	-1.8659039
H	0.1685900	1.9025374	-1.9689596
H	-0.0297918	0.0713987	-2.7210369
O	0.7147671	2.9061045	-1.6361779
H	1.2801880	3.2356654	-2.3564748
H	1.3198197	2.2526498	-0.9248893

TS4

40

Energy = -1132.169648517

C	-2.7270494	0.1213252	-0.1870665
C	-4.1853479	0.1074907	-0.1394718
C	-1.8312289	-0.1842411	0.9925682
C	-4.8481924	-0.2316379	1.0529956
C	-4.9552229	0.4249003	-1.2761749
H	-1.9518959	0.5457943	1.8002627
H	-2.0153192	-1.1806924	1.4024459
C	-0.4251020	-0.0952918	0.3787127
C	-6.2418188	-0.2549238	1.1090157
H	-4.2739116	-0.4775900	1.9414455
C	-6.3433282	0.3974663	-1.2161090
H	-4.4496942	0.6914375	-2.1990698
C	0.2380444	-1.4676727	0.2084687
N	0.4650031	0.7501926	1.1657443
C	-6.9943424	0.0581865	-0.0233479
H	-6.7380359	-0.5178135	2.0388141
H	-6.9248488	0.6431987	-2.1003011
O	-0.4074269	-2.5066986	0.1051368
N	1.6030611	-1.4282802	0.0862065
C	1.8070580	0.8107095	0.7846266
H	-8.0795206	0.0405766	0.0196225
H	2.0997629	-2.2553514	-0.2540367
C	2.4012171	-0.3032296	0.2488886
C	2.4798054	2.0375806	0.9870318
C	3.7743231	-0.5225501	-0.2321482
N	3.0099119	3.0580005	1.1799337
N	4.1521116	-1.5300090	-0.8705302
N	-2.0663213	0.4202811	-1.2612850
N	-0.7088409	0.4760258	-0.9722799
H	0.0543877	1.6371624	1.4423713
H	-0.1478181	0.1342215	-1.7502167
N	4.8337157	0.5426182	0.1687459
H	4.5850935	1.4964783	-0.1061154
H	5.7196065	0.1983701	-0.4025944
N	5.2247399	0.5791524	1.5697909
H	4.3871736	0.7730037	2.1222887
H	5.5103465	-0.3747276	1.8008656
O	6.5110886	-0.7768035	-1.2628606

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H     7.1729332   -1.2812809   -0.7623368
H     5.4302587   -1.3328518   -1.1410061
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TS5

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40
Energy = -1132.192473248
C     2.6232349    0.0945071    0.2297566
C     4.0794436    0.1045103    0.1397700
C     1.6955580   -0.1486756   -0.9388881
C     4.7112139   -0.1651668   -1.0870471
C     4.8797433    0.3761972    1.2674656
H     1.7665260    0.6474227   -1.6881400
H     1.8929648   -1.1036556   -1.4319377
C     0.3072319   -0.1452123   -0.2767016
C     6.1027663   -0.1659217   -1.1851745
H     4.1134474   -0.3749570   -1.9692590
C     6.2657177    0.3717873    1.1653362
H     4.3988422    0.5897605    2.2169637
C    -0.2702127   -1.5645550   -0.1304381
N    -0.6424011    0.7061317   -0.9757499
C     6.8852662    0.1011877   -0.0613510
H     6.5739758   -0.3754824   -2.1412401
H     6.8703236    0.5821368    2.0432223
O     0.4522492   -2.5587643   -0.0750735
N    -1.6280455   -1.6263382    0.0261967
C    -1.9744252    0.6286443   -0.6320917
H     7.9688352    0.1011458   -0.1370037
H    -2.0467177   -2.5224352    0.2672884
C    -2.4858877   -0.5444063   -0.1577829
C    -2.7710987    1.8550480   -0.7389657
C    -3.8749663   -0.7208774    0.2011617
N    -2.1898267    2.9446114   -1.0999053
N    -4.4762918   -1.6006784    0.8391898
N     1.9910467    0.3225830    1.3385873
N     0.6264809    0.3760766    1.0920238
H    -0.3320124    1.6635421   -1.1443624
H     0.0911354   -0.0050448    1.8698385
N    -4.7178362    0.4710909   -0.4559213
H    -4.8532011    0.2443121   -1.4490519
H    -5.7090287   -1.1433032    0.9654936
N    -4.1006196    1.7566721   -0.3095747
H    -4.7164451    2.4985146   -0.6355076
H    -2.8373400    3.7372374   -1.1373966
O    -6.6553751   -0.3647294    0.9623240
H    -5.6917232    0.3670280    0.0872091
H    -7.3637888   -0.7612384    0.4288812
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TS6

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43
Energy = -1208.729473728
C     2.9914485    0.0115885    0.3152919
C     4.4492298    0.0041356    0.2559563
C     2.0887234    0.2302632   -0.8777521
C     5.1044590    0.1541417   -0.9789111
C     5.2268960   -0.1584179    1.4197831
H     2.1871634    1.2453486   -1.2780673
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H	2.2840971	-0.4791655	-1.6849894
C	0.6878930	0.0177047	-0.2812542
C	6.4974605	0.1387615	-1.0507240
H	4.5243893	0.2834639	-1.8879690
C	6.6143877	-0.1758154	1.3427577
H	4.7276665	-0.2696091	2.3772643
C	0.0972415	-1.3503570	-0.6654474
N	-0.2480312	1.0601141	-0.6602389
C	7.2575255	-0.0271411	0.1074559
H	6.9872892	0.2565684	-2.0130738
H	7.2017490	-0.3032583	2.2478421
O	0.8046510	-2.3005869	-0.9935762
N	-1.2643904	-1.4562055	-0.5407175
C	-1.5777478	0.8923428	-0.4294492
H	8.3422435	-0.0392258	0.0523070
H	-1.6572672	-2.3673705	-0.7592146
C	-2.1166245	-0.3633165	-0.3455159
C	-2.4087958	2.0876965	-0.3333266
C	-3.5171377	-0.5539899	-0.0772026
N	-1.8504719	3.2562602	-0.4329767
N	-4.0883193	-1.7496285	0.0708898
N	2.3359576	-0.1489966	1.4220277
N	0.9781959	0.0295398	1.1877184
H	0.0655105	2.0296075	-0.6206542
H	0.4174209	-0.5879527	1.7718113
N	-4.2737433	0.5514904	-0.0082451
H	-5.2133224	-1.9020491	0.3345603
H	-3.4632546	-2.5381940	0.1794968
N	-3.7412765	1.8120186	-0.1877750
H	-4.4208703	2.5576045	-0.0996664
H	-2.5330593	4.0157345	-0.3696787
O	-6.5631294	-2.0168594	0.5986863
H	-5.3236399	0.5411579	0.2734341
H	-6.6564808	-2.3897509	1.4896857
O	-6.8155739	0.4564033	0.6299418
H	-6.8111402	-0.6341640	0.6786239
H	-6.9790037	0.7701801	1.5337337

TS7a

40

Energy = -1132.258944700

C	2.5278698	0.0980918	0.2744833
C	3.9745220	0.2335548	0.1424894
C	1.5733831	-0.0427614	-0.8896469
C	4.5723774	0.1923333	-1.1292446
C	4.7983378	0.3990557	1.2735524
H	1.5455220	0.8649722	-1.5027823
H	1.8251544	-0.8860481	-1.5367299
C	0.2236184	-0.2665646	-0.1902777
C	5.9553458	0.3098319	-1.2682558
H	3.9555449	0.0677087	-2.0144647
C	6.1758851	0.5132942	1.1300632
H	4.3426989	0.4363520	2.2581368
C	-0.2233029	-1.7366540	-0.2511415
N	-0.8328007	0.5736313	-0.7396674
C	6.7620466	0.4694523	-0.1411943

H	6.4006702	0.2761219	-2.2584262
H	6.7998673	0.6393393	2.0104790
O	0.5659579	-2.6589830	-0.4322690
N	-1.5562870	-1.9437702	0.0031592
C	-2.1287786	0.3449665	-0.3372844
H	7.8390361	0.5609003	-0.2484860
H	-1.8730687	-2.9097858	0.0340722
C	-2.5052217	-0.9240696	0.0509094
C	-3.1428502	1.3522256	-0.3817778
C	-3.8475209	-1.1824708	0.4558188
N	-2.9960509	2.6334705	-0.7279558
N	-4.2202834	-2.4760748	0.8110346
N	1.9263172	0.1092326	1.4225803
N	0.5505817	0.0845065	1.2262291
H	-0.5603546	1.5402774	-0.8879893
H	0.0827213	-0.4501739	1.9555557
N	-4.7757387	-0.2450806	0.4189846
H	-5.1892386	-2.5234975	1.1160737
H	-3.6150841	-2.9159682	1.5004099
N	-4.3927425	0.9670613	-0.0271388
H	-5.1146777	1.7587131	-0.1436543
H	-2.1358971	2.9341031	-1.1663580
O	-5.4030153	3.3077667	-0.5550879
H	-4.0318185	3.1640283	-0.7723028
H	-5.8540148	3.3390088	-1.4141918

TS7

43

Energy = -1208.751673345

C	2.8213261	0.1252748	0.2750375
C	4.2539865	0.3686430	0.1443787
C	1.8758475	-0.0581669	-0.8907854
C	4.8495536	0.4012751	-1.1286404
C	5.0670779	0.5651635	1.2782639
H	1.7741301	0.8624920	-1.4763775
H	2.1897080	-0.8594152	-1.5633572
C	0.5522556	-0.4080870	-0.1938826
C	6.2201410	0.6212023	-1.2661548
H	4.2408576	0.2544005	-2.0160707
C	6.4324172	0.7817032	1.1361850
H	4.6129625	0.5455068	2.2640319
C	0.2322147	-1.9085018	-0.2803601
N	-0.5737959	0.3490745	-0.7270989
C	7.0165830	0.8105468	-0.1364071
H	6.6641329	0.6434519	-2.2572242
H	7.0481304	0.9304428	2.0188516
O	1.0938408	-2.7579756	-0.4833905
N	-1.0772498	-2.2293517	-0.0213478
C	-1.8468620	0.0091574	-0.3260801
H	8.0839658	0.9813633	-0.2426661
H	-1.3135268	-3.2184904	-0.0047114
C	-2.1065772	-1.2938162	0.0449825
C	-2.9474410	0.9254454	-0.3600707
C	-3.4172562	-1.6654076	0.4537488
N	-2.8264083	2.2024676	-0.7501203
N	-3.6851890	-2.9864769	0.7954252

N	2.2236780	0.0676762	1.4237037
N	0.8524370	-0.0551793	1.2277864
H	-0.3705588	1.3324704	-0.8723785
H	0.4284846	-0.6383066	1.9469199
N	-4.4164659	-0.8048033	0.4318871
H	-4.6445281	-3.1149069	1.1070356
H	-3.0387105	-3.3922176	1.4677109
N	-4.1556902	0.4475311	-0.0017141
H	-5.0628393	1.0863602	-0.0630453
H	-1.9187874	2.5434054	-1.0291655
O	-6.2474634	1.9826543	-0.1323776
H	-5.6059002	3.0239784	-0.3086192
H	-6.7418127	1.8052315	-0.9481581
O	-4.8316184	3.9381277	-0.4865981
H	-3.6159310	2.9264847	-0.6441750
H	-4.7420364	4.3951969	0.3646697

TS8^{+}

38

Energy = -1056.205637506

C	2.1185005	-0.2609830	0.3767912
C	3.5116916	0.1204354	0.1993954
C	1.3510398	-1.2132273	-0.5213801
C	4.2594833	-0.4248127	-0.8583185
C	4.1278752	1.0282974	1.0827636
H	1.4507630	-1.0298950	-1.5914623
H	1.6557758	-2.2504204	-0.3308381
C	-0.0487862	-1.0235532	0.0112529
C	5.5975525	-0.0751157	-1.0267069
H	3.8000365	-1.1267735	-1.5477628
C	5.4614767	1.3748331	0.9073297
H	3.5516508	1.4527602	1.8985352
C	-1.0711258	-2.1507739	-0.0539451
N	-0.8202941	0.2331101	-1.1525952
C	6.2009480	0.8244554	-0.1464795
H	6.1672811	-0.5047189	-1.8449099
H	5.9300591	2.0758543	1.5914730
O	-0.7052191	-3.3147062	-0.0862649
N	-2.3865225	-1.7707075	0.0128408
C	-2.1312399	0.5464366	-0.6534909
H	7.2432102	1.0986999	-0.2793625
H	-3.0631475	-2.5309241	0.0482821
C	-2.8660331	-0.4591127	-0.0656191
C	-2.6490455	1.8545900	-0.6910900
C	-4.1292989	-0.0992869	0.4766542
N	-3.8369759	2.1340403	-0.1436977
N	-4.5544397	1.1681126	0.4441844
N	1.3928819	0.1479211	1.3780765
N	0.1298709	-0.4298145	1.2197475
H	-0.8304224	-0.1718237	-2.0935538
H	-0.5782606	-0.2286280	1.9146951
N	-1.8961935	2.8913705	-1.2186457
H	-2.3894042	3.7804448	-1.1941125
H	-1.5093894	2.7249351	-2.1437253
N	-4.9756680	-1.0538504	0.9993044
H	-4.5481546	-1.7856008	1.5580579

H -5.7901701 -0.6573683 1.4596709
H -0.2248936 1.0676757 -1.1572425

TS9
37
Energy = -1055.754181071
C 2.6437937 -0.6549891 -0.3205982
C 3.9273665 0.0168806 -0.2061537
C 1.3422347 -0.1934490 0.2531137
C 4.0397975 1.2138234 0.5248391
C 5.0744192 -0.5217154 -0.8234819
H 1.3510456 -0.0828103 1.3435512
H 1.0219035 0.7711075 -0.1654906
C 0.4693258 -1.3052576 -0.2174461
C 5.2685323 1.8574603 0.6373498
H 3.1648014 1.6389151 1.0075106
C 6.2984550 0.1252764 -0.7082290
H 4.9866043 -1.4441967 -1.3877183
C -0.9747804 -1.4727582 0.0152244
N -4.2990402 -1.5138877 0.4634119
C 6.3997110 1.3151360 0.0219409
H 5.3456152 2.7800734 1.2043784
H 7.1783274 -0.2944809 -1.1864792
O -1.6301183 -2.3640837 -0.5044510
N -1.5552587 -0.4735849 0.9017311
C -3.9330569 -0.2272506 0.1478804
H 7.3584317 1.8176212 0.1102924
H -1.8334244 -0.9312435 1.7734624
C -2.6522577 0.2769706 0.3346661
C -4.9061469 0.6926523 -0.3584552
C -2.4158085 1.6266691 -0.0170337
N -4.6076203 1.9358900 -0.6998674
N -3.3542141 2.4178265 -0.5462516
N 2.4907114 -1.7855177 -0.9818005
N 1.1457338 -2.1811224 -0.9134460
H -3.5407222 -2.1904144 0.3989107
N -6.2091787 0.2359447 -0.5959494
H -6.8103440 0.9945883 -0.9103732
H -6.6349741 -0.2294994 0.2035708
N -1.1476852 2.1715035 0.1445548
H -0.6539228 1.7752549 0.9386608
H -1.1549812 3.1872016 0.1508302
H -5.1454671 -1.8398856 0.0073827

TS9^{+}
38
Energy = -1056.182973600
C 2.5690027 -0.7790300 0.0432110
C 3.7106374 0.0968466 -0.1250604
C 1.1446493 -0.4287755 -0.2735730
C 3.5148578 1.4312877 -0.5260964
C 5.0174033 -0.3730819 0.1159767
H 0.7057597 0.4098111 0.3281260
H 0.9858553 -0.1354050 -1.3184743
C 0.4640864 -1.6957713 0.0693290
C 4.6048010 2.2810460 -0.6807836

H	2.5125927	1.8048642	-0.7130911
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H	7.1060630	0.1177840	0.1438988
O	-1.5261741	-2.6549982	-0.7877788
N	-1.6615777	-1.1333481	1.0077475
C	-3.7168806	-0.2129750	-0.0618773
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H	-1.9149163	-1.6022147	1.8754335
C	-2.4789966	-0.0430614	0.5472106
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C	-1.9733803	1.2690985	0.6853462
N	-3.8150855	2.1907549	-0.3663390
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H	-5.9951004	1.8098558	-1.3430755
H	-6.2740961	0.2923568	-0.6949411
N	-0.7213473	1.4793304	1.2799518
H	-0.5805502	0.9284684	2.1233611
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H	-5.0286637	-1.4710635	-0.9717765

X-Ray crystallographic details for compounds 1a, 2a and 3a.

General Information

The X-ray diffraction data for the crystals of compounds **1a**, **2a** and **3a** were collected on a Bruker D8 Quest single crystal X-ray diffractometer equipped with an Incoatec IμS microfocus source (Mo Kα, λ = 0.71073 Å), a multilayers optics monochromator, and a PHOTON III area detector, in the ω and φ-scan modes at 100(2) K for **1a**, 162(2) K for **2a** and 150(2) K for **3a** samples. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method by SADABS program.[1] The structures were solved by direct method using SHELXS and refined by the full matrix least-squares using SHELXTL programs.[2] Data collection: images were indexed and integrated using the APEX3 data reduction package.[3] All calculations were performed on PC using WinGX suit of programs.[4] All non-hydrogen atoms were refined with individual anisotropic displacement parameters for all compounds. The hydrogen atoms were inserted at calculated positions and refined as riding atoms except the hydrogen atoms on amino-groups and hydrogen atoms of water molecule, which were determined based on the electronic density distribution from and were refined isotropically.

The geometry of the compounds **1a**, **2a** and **3a** was established by X-ray diffraction analysis of the single crystals. Detail of refinement procedures and crystal parameters are presented in Table S1 (see ESI) and peculiarity of hydrogen bonding and crystal packing are shown on the figures S1-S3. Compound **1a** form monoclinic crystals (space groups *P21/c*) and crystalize individually (Figure S1). Molecule **1a** practically planar within experimental errors and this leads to a significant influence of π-electron contacts between aromatic fragments of planar molecule, along with classical hydrogen bonds of N-H…O type, on their packing in the crystal (Figure S1).

In contrast to the previous compound, products **2a** and **3a** does not crystallize individually but forms mixed solvate with DMF and water in a 2:2:1 stoichiometric ratio (Figure S2) in the case of **2a**, and solvate with DMF in ratio 1:2 in the case of **3a** compound (Figure S3). The main structure-forming interactions in the crystals of both compounds leads to the formation of porous supramolecular structures in crystals. The solvate water molecules in **2a** crystals is situated at special positions and participate, along with classical N-H…N hydrogen bonds between **2a** molecules, in formation of H-bonded layered 2D-structures (Figures 4S). But the solvate DMF molecules in the crystals of both compounds **2a** and **3a** concentrated into the 1D-porous channels (Figures 5S and 6S).

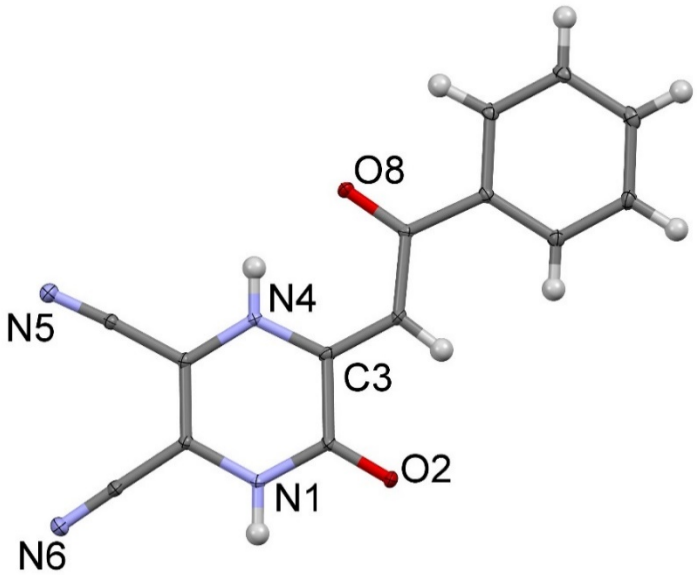

Figure S1. Molecular structure of **1a (MVA2023_16F)** and partial numbering scheme. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres.

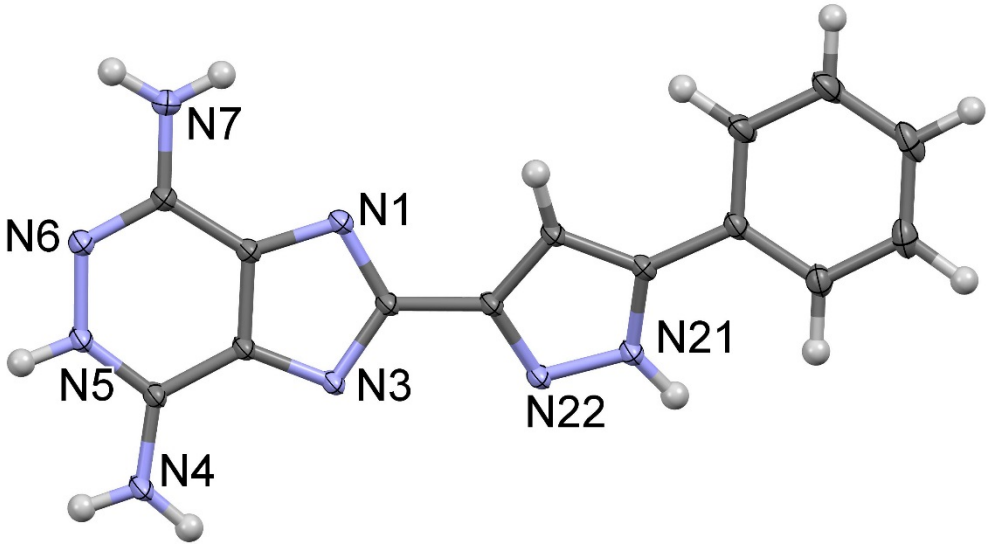

Figure S2. Molecular structure of **2a (MVA2022_47)**. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres. Solvate water and DMF molecules are not shown.

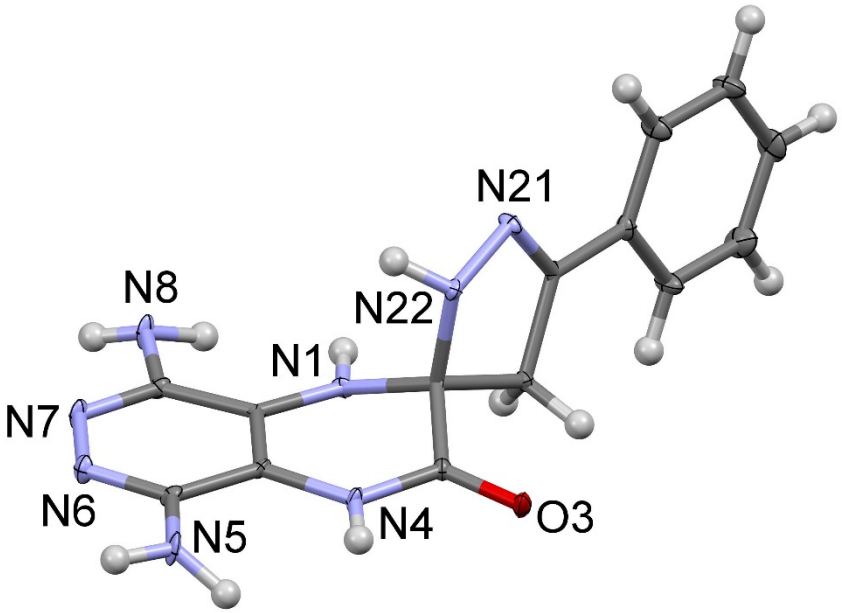

Figure S3. Molecular structure of **3a (MVA2023_54)**. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres. Two solvate DMF molecules are not shown.

Analysis of the intermolecular interactions was performed using the program PLATON.[5] The Mercury program package[6] was used for molecular graphics. The crystal data, data collection, and the refinement parameters are given in Tables S1.

Crystallographic data (excluding structure factors) for the investigated structures **1a**, **2a** and **3a** have been deposited in the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC **2373968-2373970**, respectively. Copies of the data can be obtained free of charge upon application to the CCDC (12 Union Road, Cambridge CB2 1EZ UK. Fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk).

Table 1S. Parameters of X-ray diffraction experiments for compounds 1**a**, **2a** and **3a.**

Compound, Formula	**1a_MVA2023_16f** $C_{14}H_8N_4O_2$	**2a_MVA2022_54f** $2(C_{14}H_{12}N_8)$, $2(C_3H_7NO)$, H_2O	**3a_MVA2023_47f** $C_{14}H_{14}N_8O$, $2(C_3H_7NO)$
M (g/mol)	264.24	748.84	456.52
Temperature, K	100(2)	162(2)	150(2)
Crystal class	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$C2/c$	$P2_1/n$
Crystal size	0.014×0.084×0.383 mm^3	0.134×0.201×0.263 mm^3	0.024×0.208×0.332 mm^3
Z, Z′	4, 1	4, 1	4, 1
Cell parameters	a= 13.1843(14)Å b= 12.8448(14)Å c= 6.8879(7)Å β= 94.584(4)°	a= 24.826(3)Å b= 10.5319(13)Å c=16.192(2) Å β=117.179(4) °	a= 13.4925(9)Å b= 8.4402(5)Å c= 20.7218(14)Å β= 103.011(3)°
V, Å^3	1162.7(2) Å^3	3766.2(8)Å^3	2299.2(3) Å^3
F(000)	544	1576	968
ρ_{calc}, g/cm^3	1.510	1.321	1.319
μ, cm^{-1}	1.06	0.92	0.94
θ, deg	2.217≤ θ ≤ 29.127	1.844≤ θ ≤ 34.804	2.030≤ θ ≤ 29.170
Refl. measured	20407	84574	23075
Independ. refl. / R_{int}	2953 / 0.0454	8114 / 0.0695	6059 / 0.1015
Param. / restraints	198 / 0	329 / 0	331 / 0
Reflections [I>2σ(I)]	2757	6405	4120
R_1 / wR_2 [I>2σ(I)]	0.0986 / 0.2134	0.0484 / 0.1318	0.1221 / 0.2046
R_1 / wR_2 (all refl.)	0.1033 / 0.2157	0.0613 / 0.1438	0.1777 / 0.2222
Goodness-of-fit on F^2	1.170	1.042	1.173
ρ_{max}/ρ_{min} (eÅ^{-3})	0.520 / -0.497	0.473 / -0.242	0.458 / -0.398

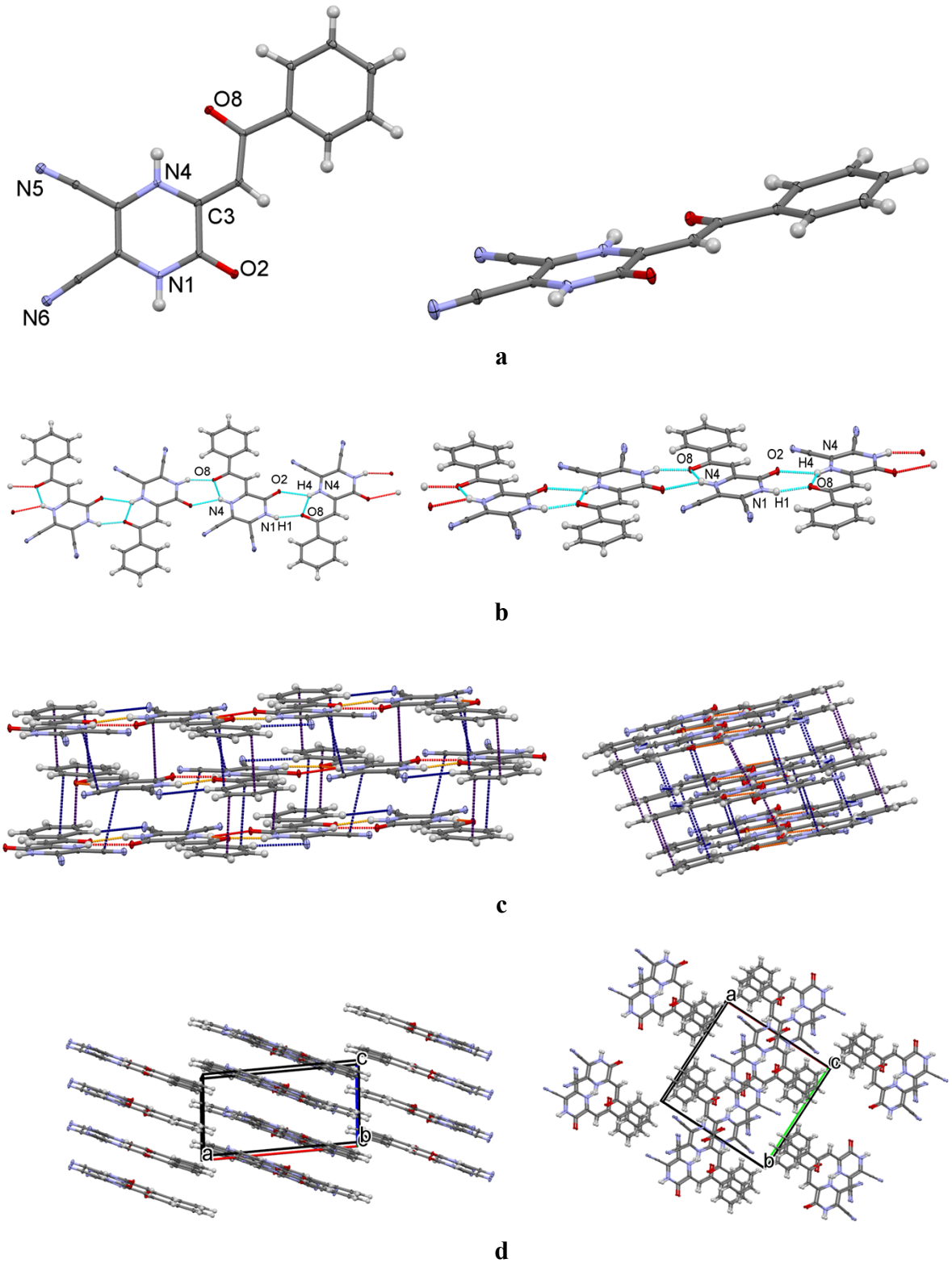

Figure S4. (a) Two projections of the molecule in the crystal of **1a**. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres; (**b**) two projections of one-dimensional chain of bounded by N-H…O interactions molecules along *0b* axis in the crystal of **1a**, H-bonds are shown by blue dashed lines; (**c**) 3D-supramolecular structure, formed in **1a** crystal owing to combined action of N-H…O bonds and π…π contacts; (**d**) two projection of crystal packing in the crystal of **1a**.

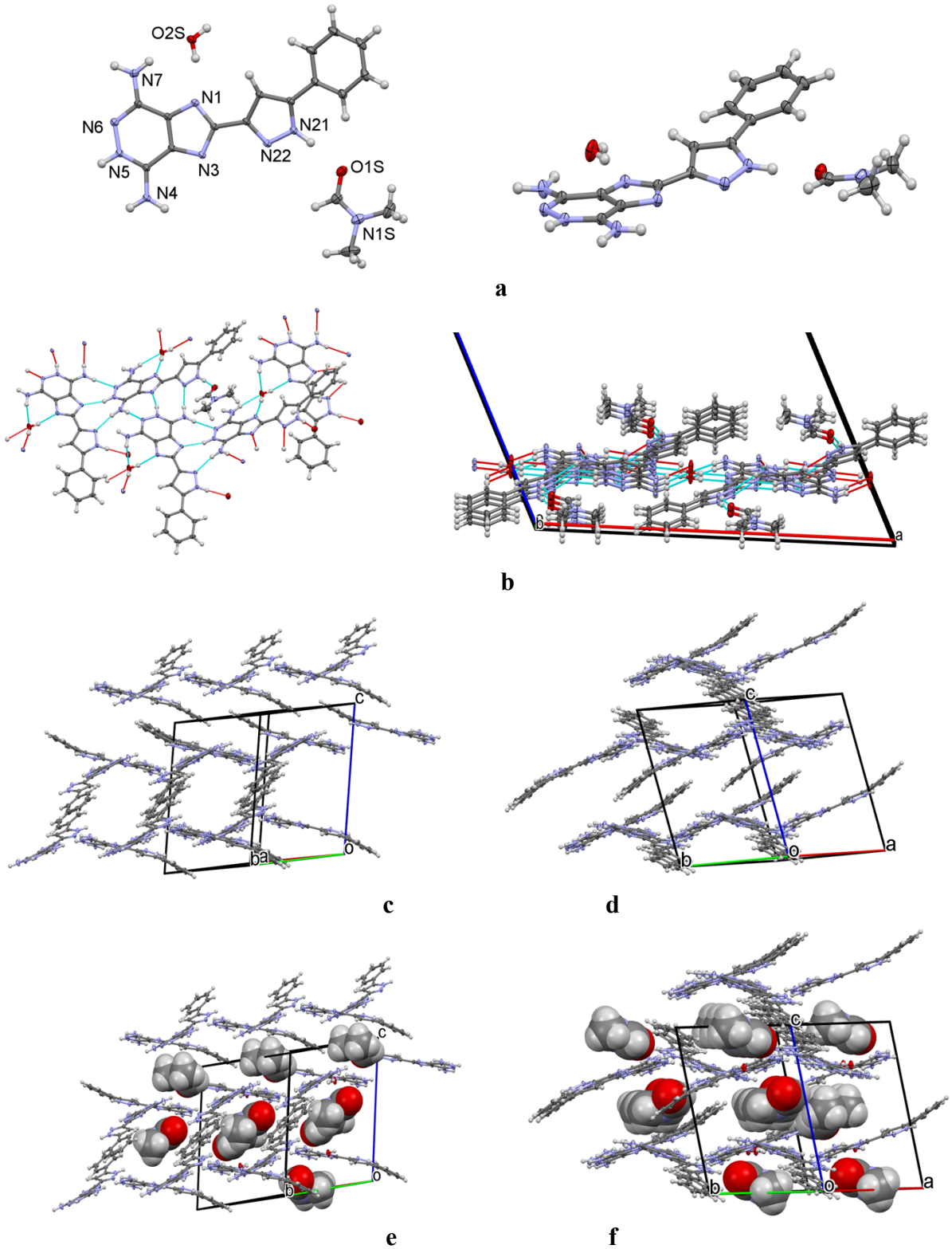

Figure S5. (**a**) Two projections of the molecule in the crystal of **2a** with partial numbering scheme. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres; (**b**) two projections of 2D-supramolecular structure in the crystal of **2a** - H-layers along *a0b* plane of bounded by N-H…O, N-H…N and O-H…N interactions molecules (H-bonds are shown by blue and red dashed lines); (**c, d**) two projections of the porous structure in the crystal **2a**, formed owing to H-bonding between **2a** and water molecules. Solvate acetic acid molecules are not shown; (**e, f**) the same, but with solvate DMF molecules (in space-fill model representation) in porous 1D-chanels.

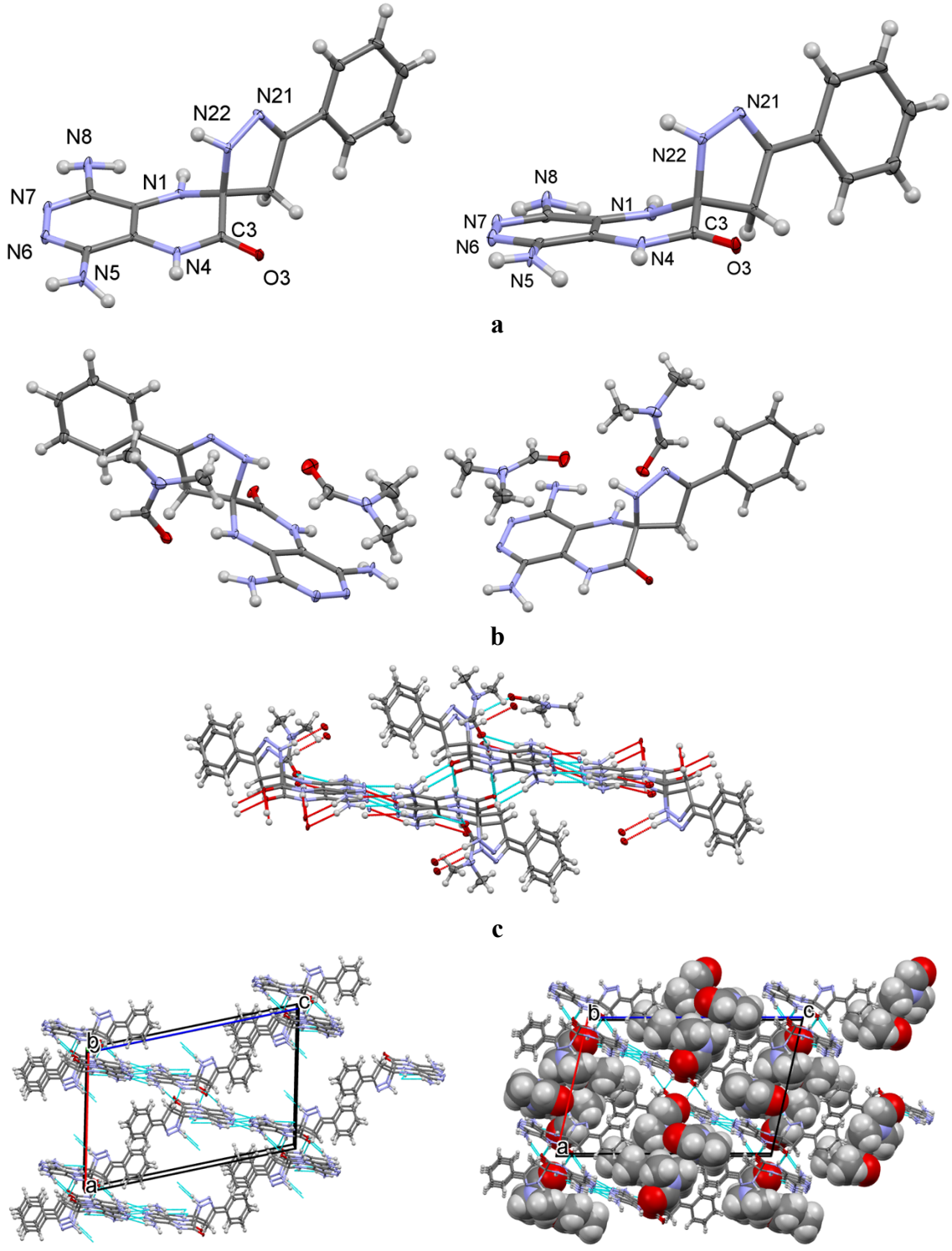

Figure S6. (**a**) Two projections of the molecule in the crystal of **3a** with partial numbering scheme. Displacement ellipsoids are drawn at the 30% probability level; hydrogen atoms are represented as fixed-size spheres; (**b**) two projections of the molecule in the crystal of **3a** with solvate DMF molecules; (**c**) fragment of H-bonding of **3a** and DMF molecules in the crystal, H-bonds are shown by blue and red dashed lines; (**d**) 3D-supramolecular porous structure, formed in **3a** crystal owing to H-bonding only between **3a** molecules. Solvate DMF molecules are not shown; (**e**) the same, but DMF molecules included in the 1D-pores (along *0b* axis) and are shown in space-fill model.

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2. G. Sheldrick, SHELXTL v.6.12, Structure Determination Software Suite, Bruker AXS, Madison, Wisconsin, USA, 2000.

3. APEX2 (Version 2.1), SAINTPlus, Data Reduction and Correction Program (Version 7.31A), BrukerAXS Inc., Madison, Wisconsin, USA, 2006.

4. L. J. Farrugia, WinGX suite for small-molecule single-crystal crystallography, *J. Appl. Crystallogr.*, 1999, **32**, 837.

5. A. L. Spek, Single-crystal structure validation with the program PLATON. *J. Appl. Crystallogr.* 2003, **36**, 7−13.

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