Supporting Information for "Structural and spectroscopic aspects of $SCN^{(-)}(H_2O)_n$ clusters and the temperature dependency of the isomers: A parallel tempering based approach"

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Keywords: Thiocyanate-water clusters, Parallel Tempering, Molecular Clusters, Quantum Chemical Calculations, Temperature dependency of isomers.

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FIGURES

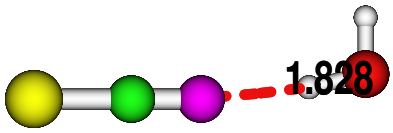
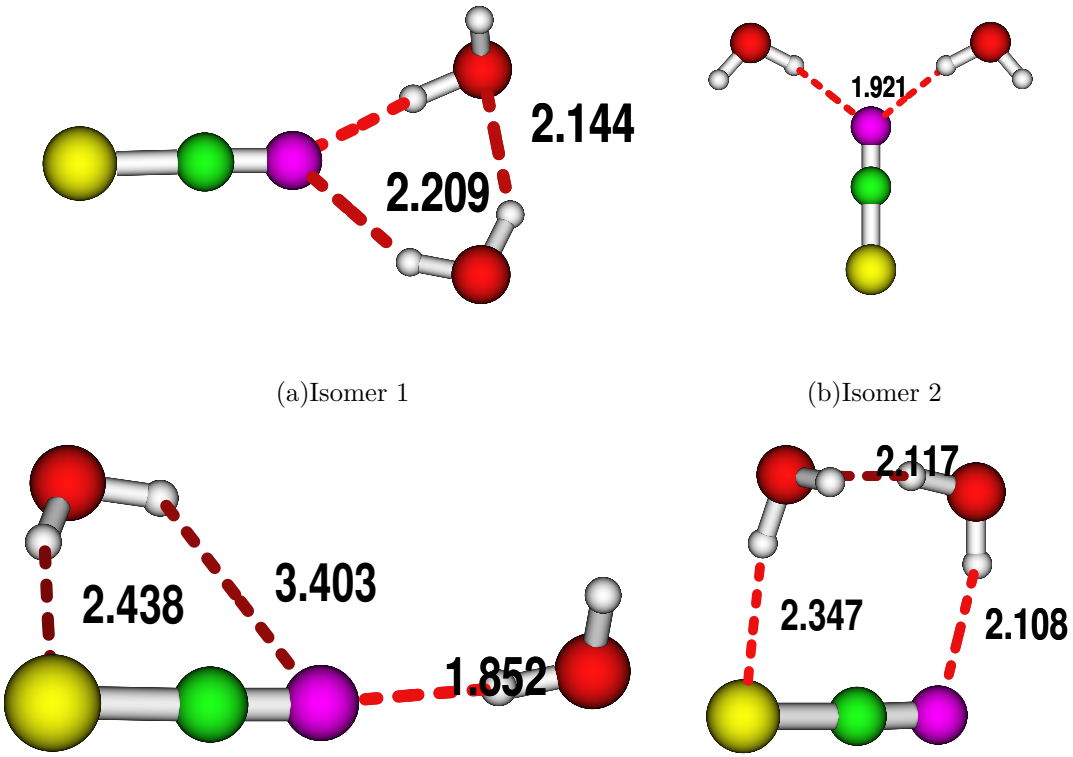


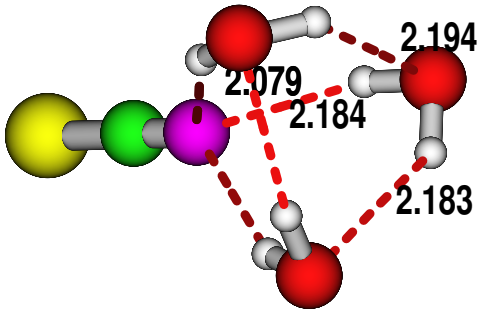
FIG. 1. Optimized structure of $SCN^{(-)}H_2O$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atom is shown in yellow, C atom is shown in green, N atom is shown in pink and O and H atoms are shown in red and gray respectively.



(a)Isomer 1 (b)Isomer 2

(c)Isomer 3 (d)Isomer 4

FIG. 2. Optimized structure of $SCN^{(-)}(H_2O)_2$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



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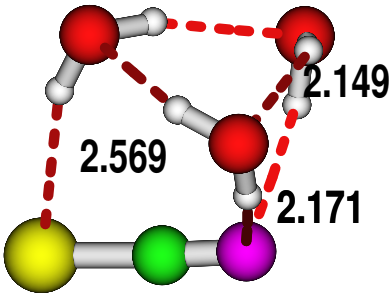

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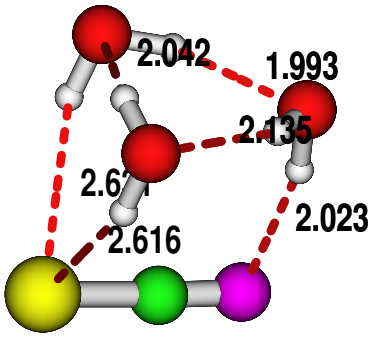
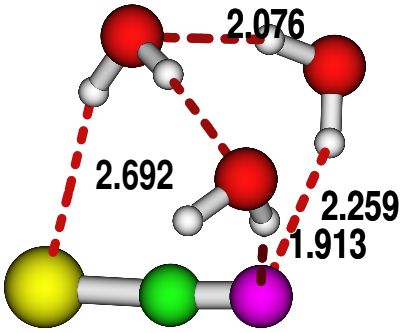


(c)Isomer 3



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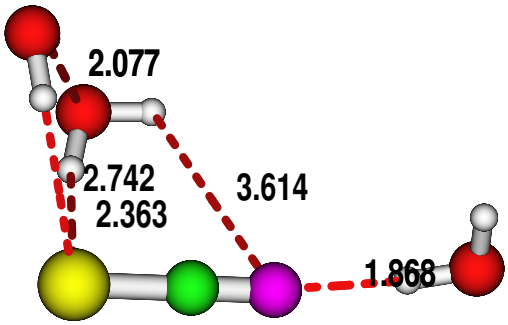

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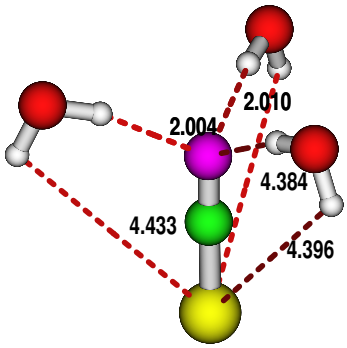

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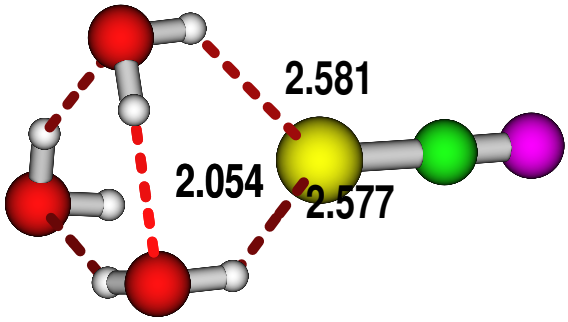
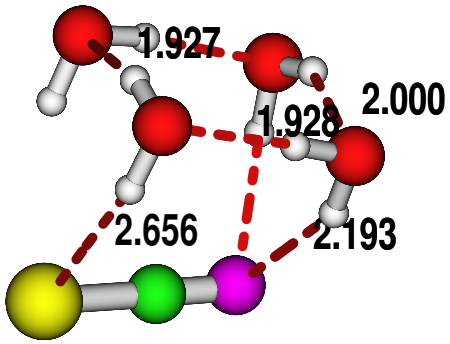


(g)Isomer 7

FIG. 3. Optimized structure of $SCN^{(-)}(H_2O)_3$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



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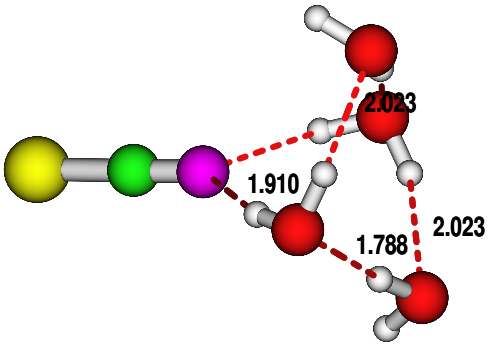

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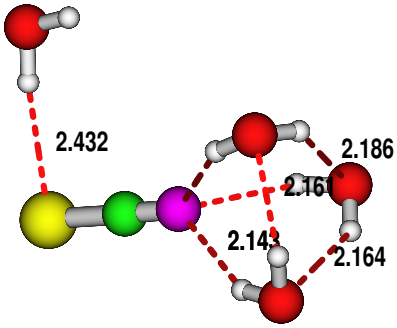

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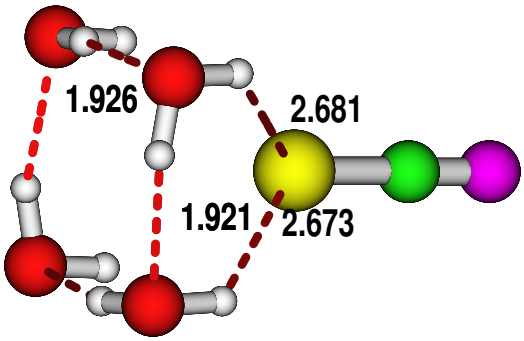

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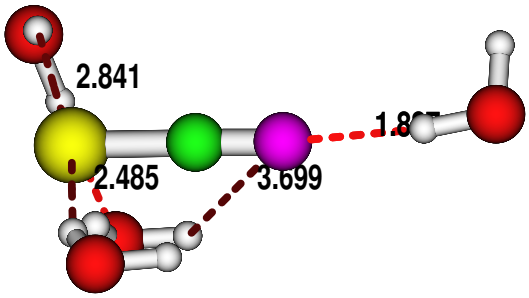

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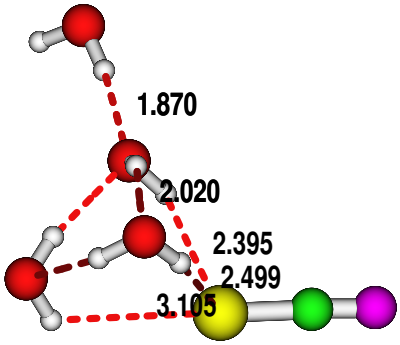
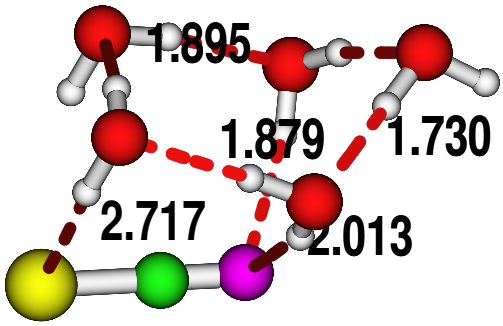


(f)Isomer 6

FIG. 4. Optimized structure of $SCN^{(-)}(H_2O)_4$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



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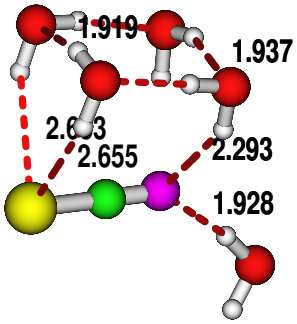

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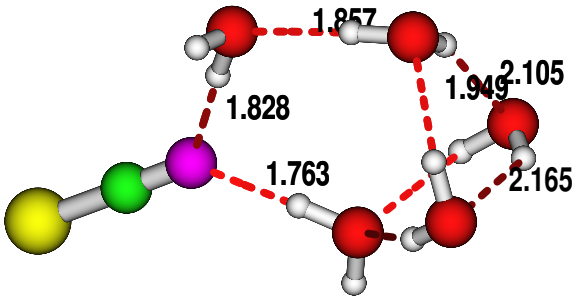

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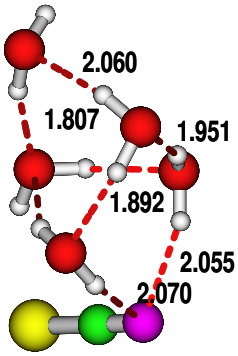

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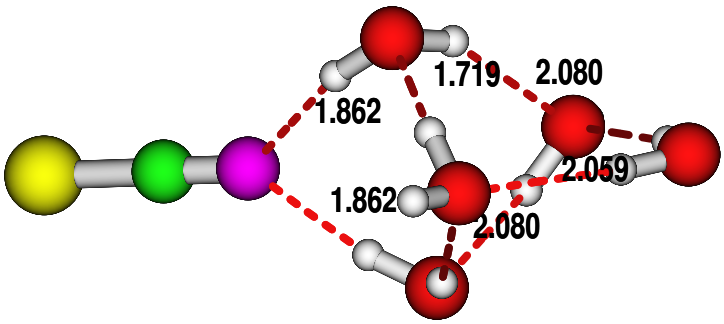

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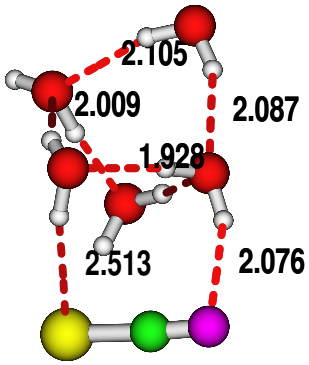

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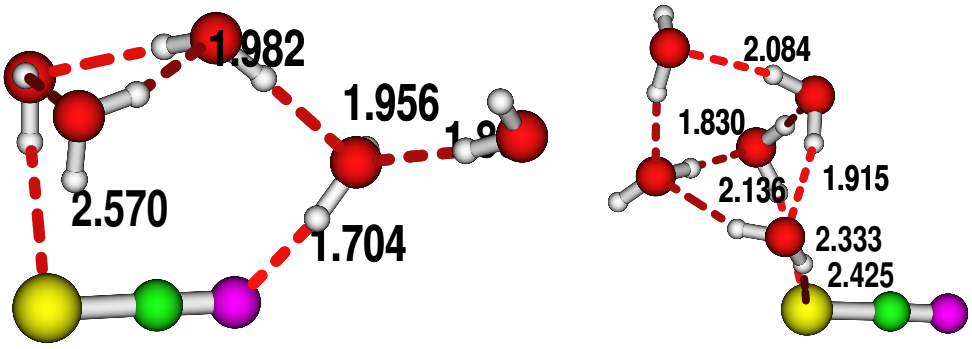
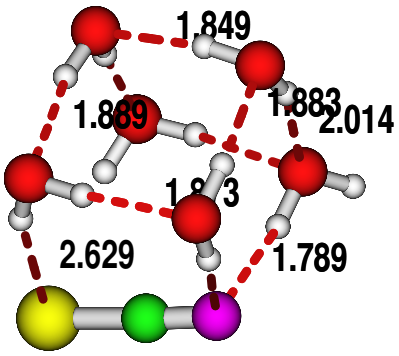


(g)Isomer 7 (h)Isomer 8

FIG. 5. Optimized structure of $SCN^{(-)}(H_2O)_5$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



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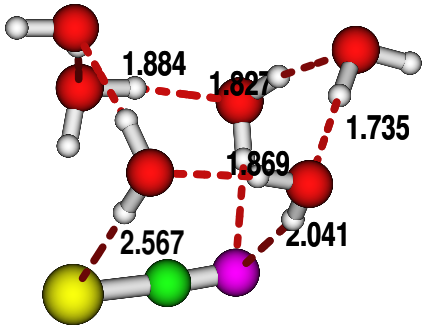

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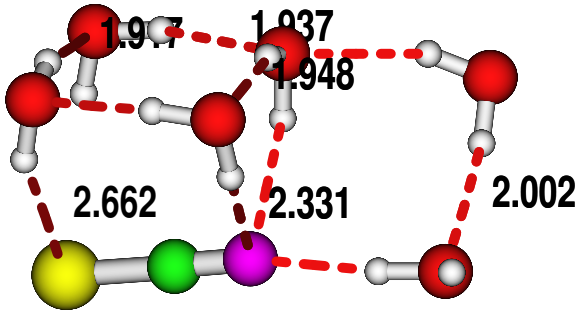

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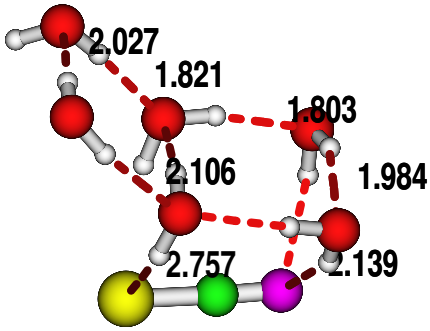

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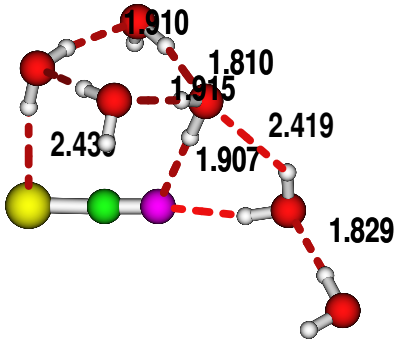

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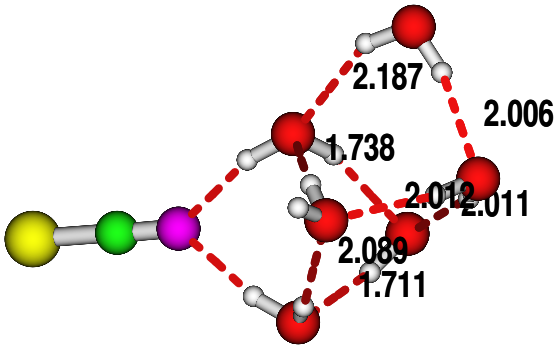

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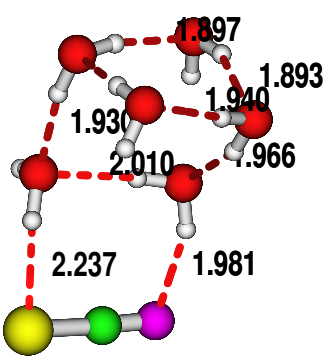

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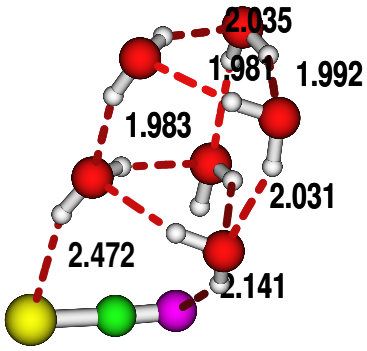

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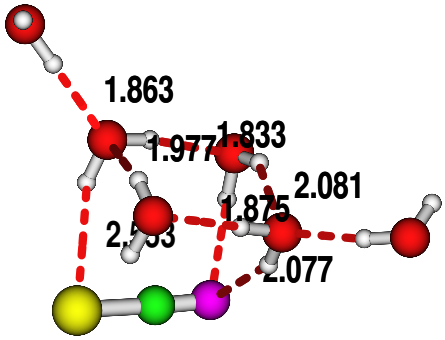

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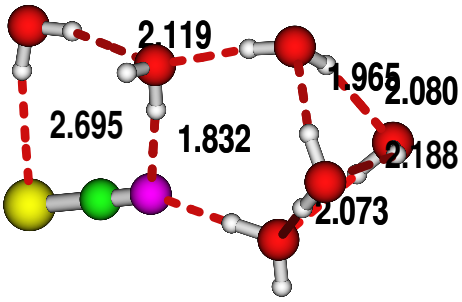

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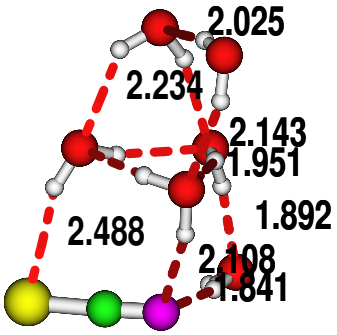

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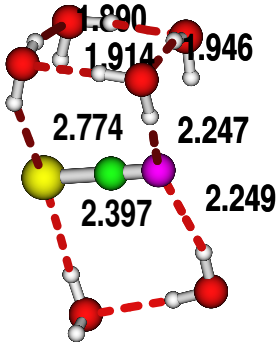

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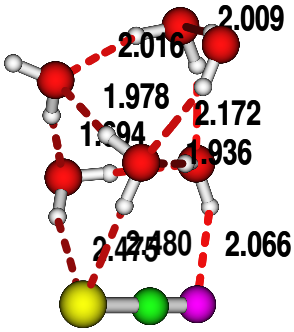

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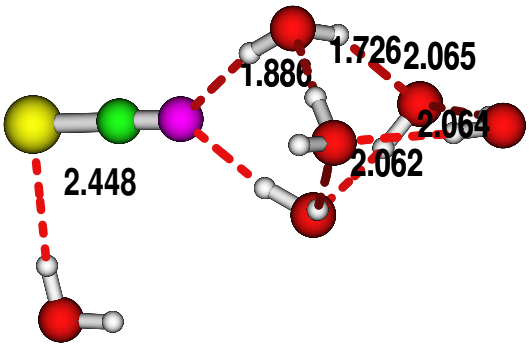

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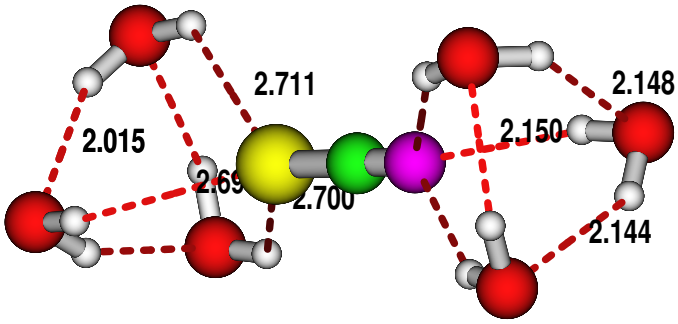

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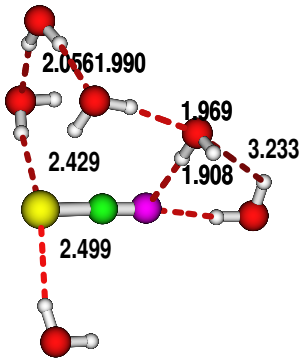

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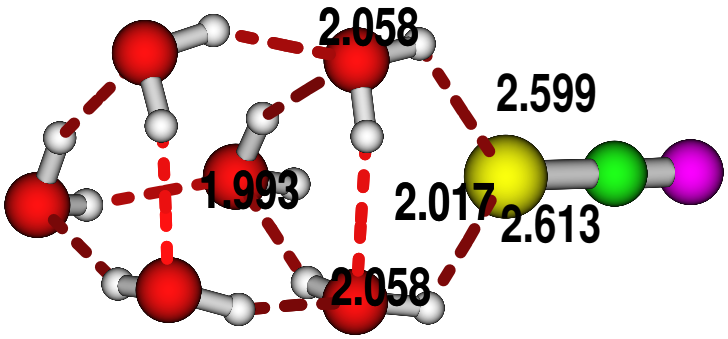

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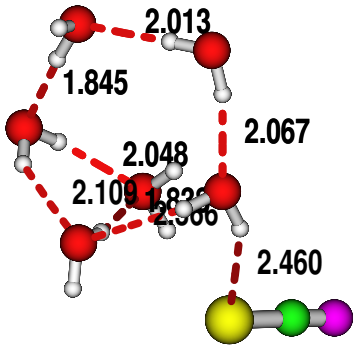
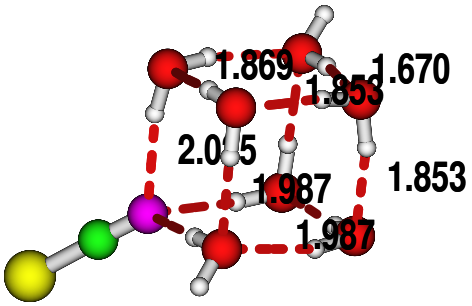


(r)Isomer 18

FIG. 6. Optimized structure of $SCN^{(-)}(H_2O)_6$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



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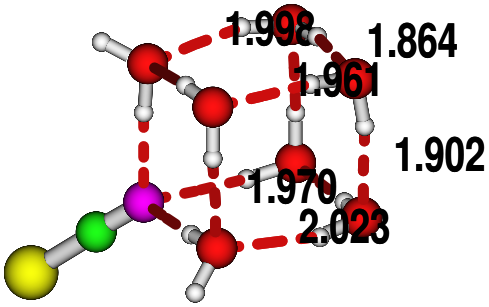

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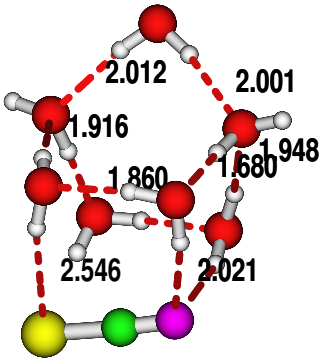

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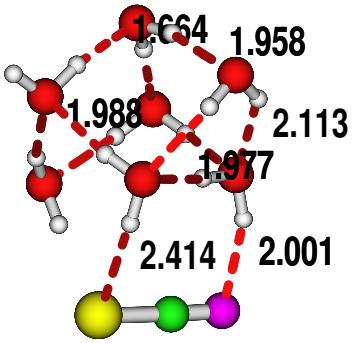

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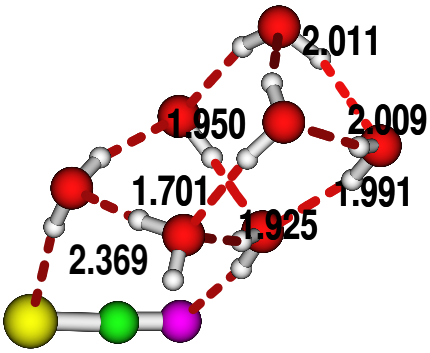

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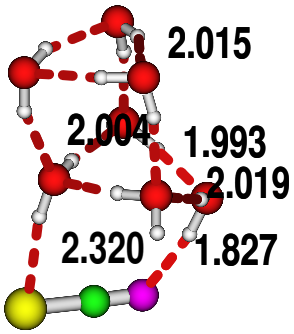

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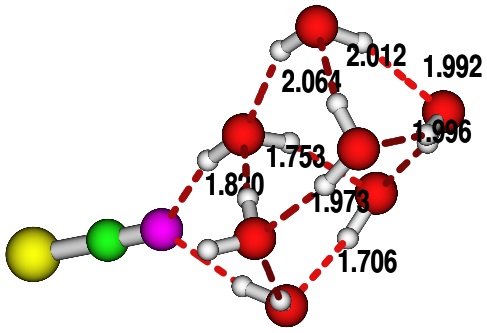

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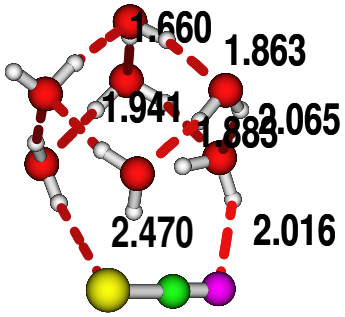

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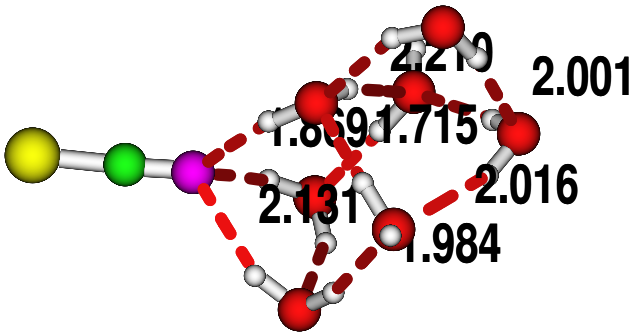

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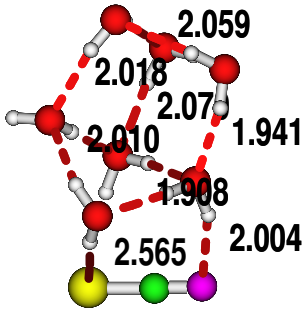

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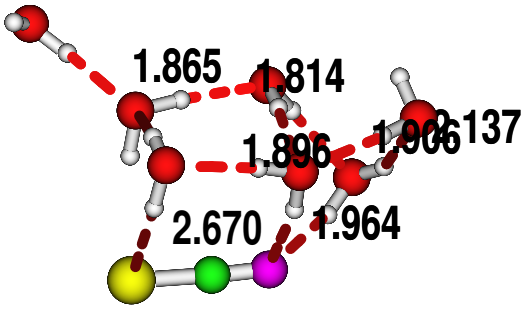

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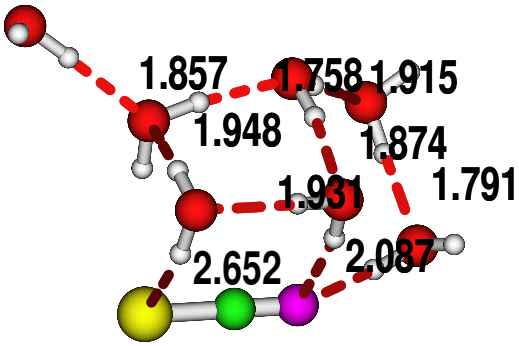

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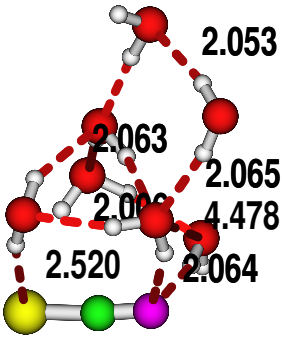

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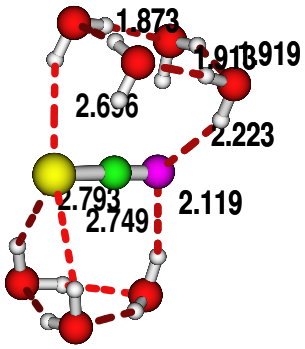
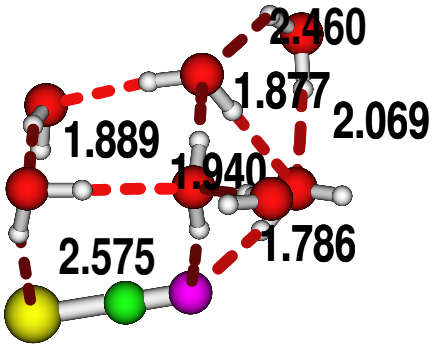
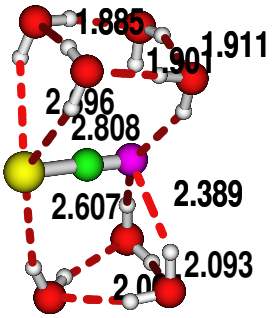


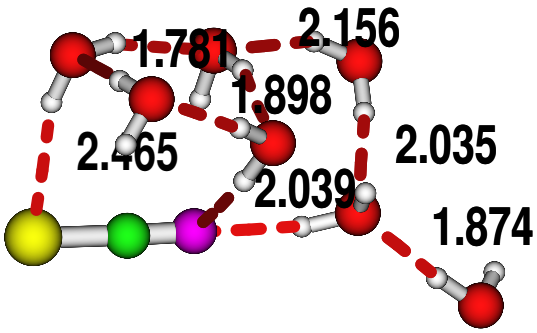
(n)Isomer 14



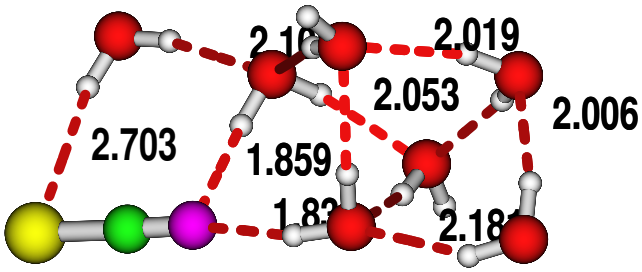
(o)Isomer 15



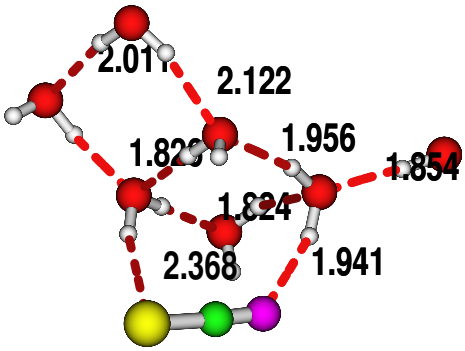
(p)Isomer 16



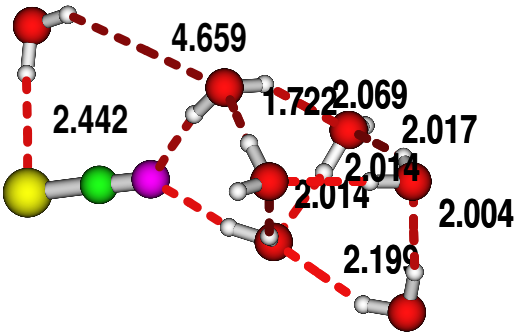
(q)Isomer 17



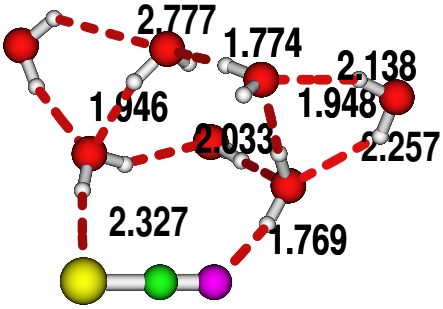
(r)Isomer 18



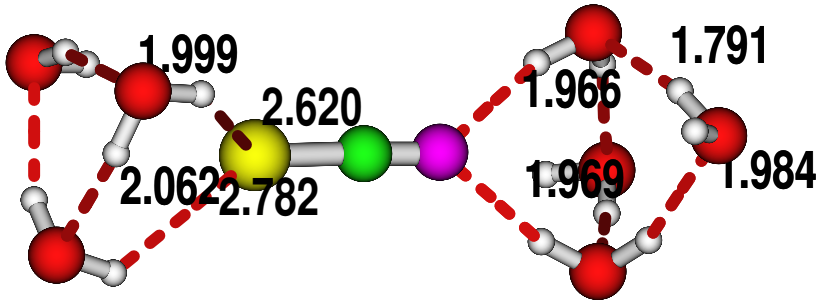
(s)Isomer 19



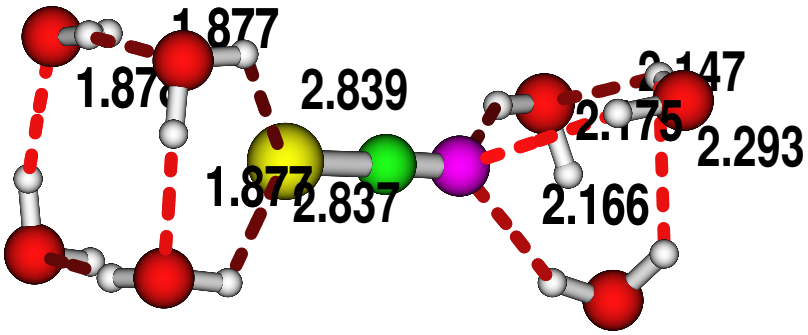
(t)Isomer 20



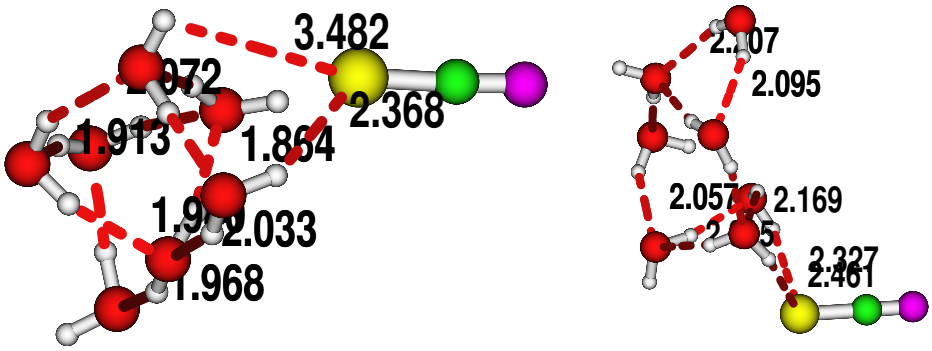
(u)Isomer 21



(v)Isomer 22

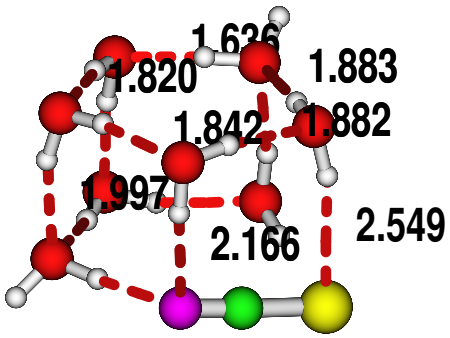


(w)Isomer 23

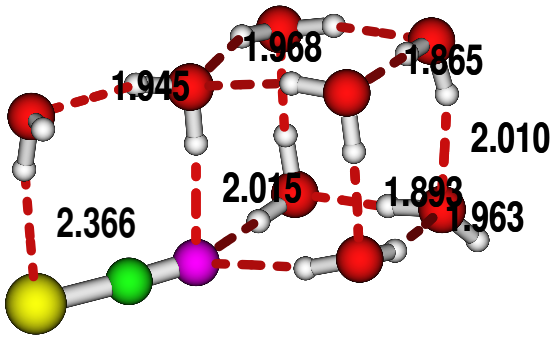


(x)Isomer 24 (y)Isomer 25

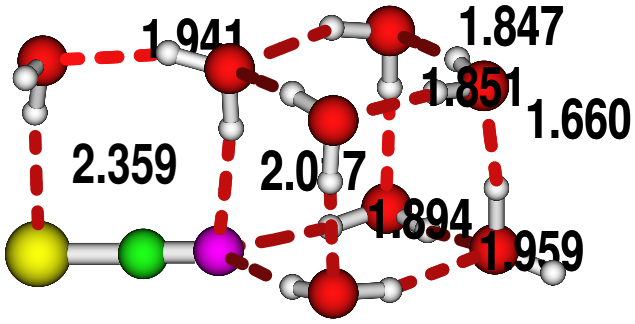
FIG. 7. Optimized structure of $SCN^{(-)}(H_2O)_7$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



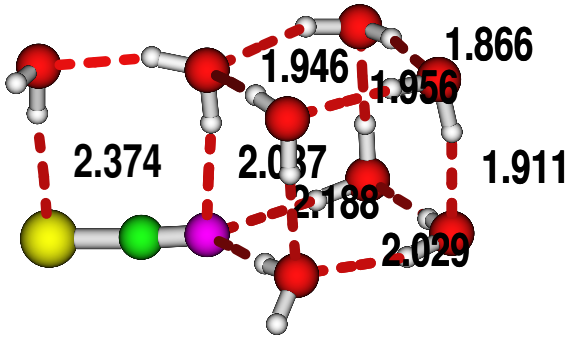
(a)Isomer 1



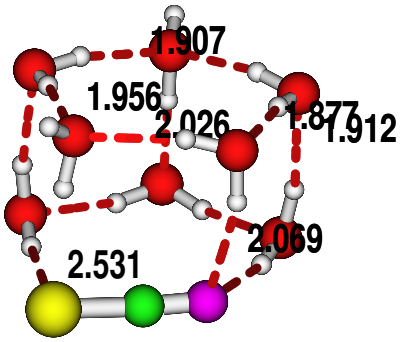
(b)Isomer 2



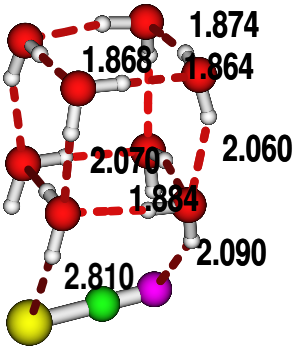
(c)Isomer 3



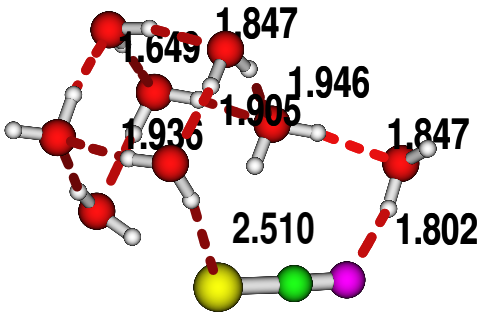
(d)Isomer 4



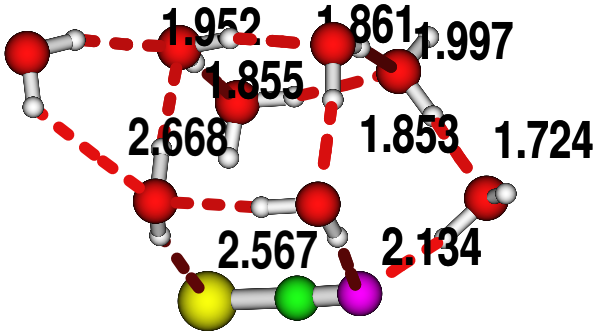
(e)Isomer 5



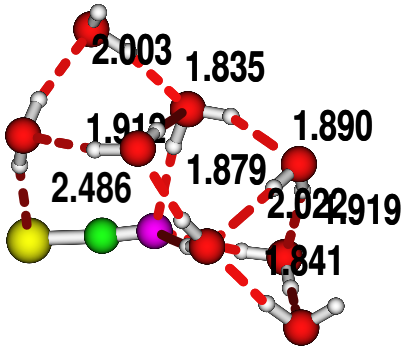
(f)Isomer 6



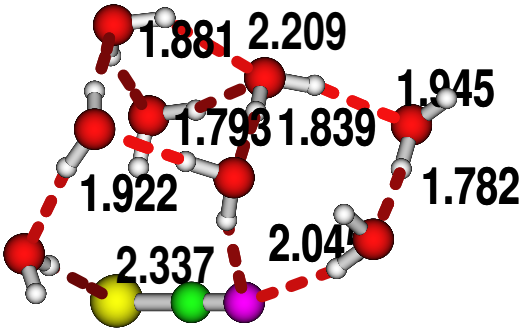
(g)Isomer 7



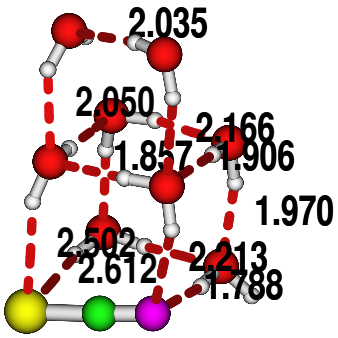
(h)Isomer 8



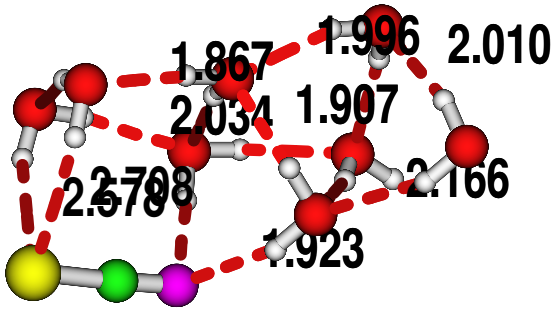
(i)Isomer 9



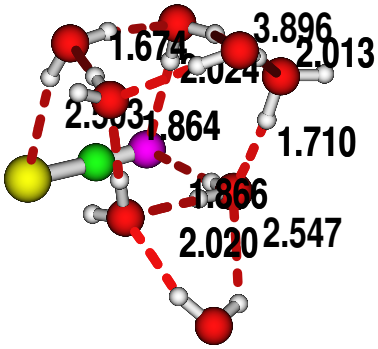
(j)Isomer 10



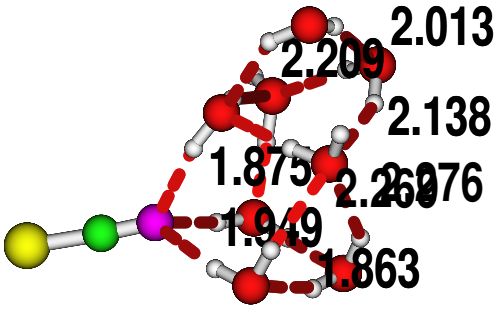
(k)Isomer 11



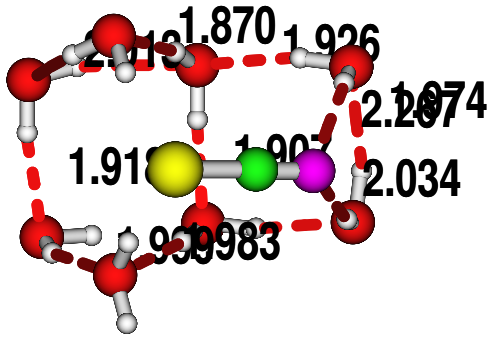
(l)Isomer 12



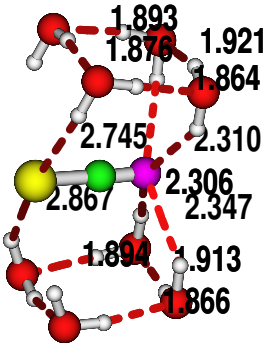
(m)Isomer 13



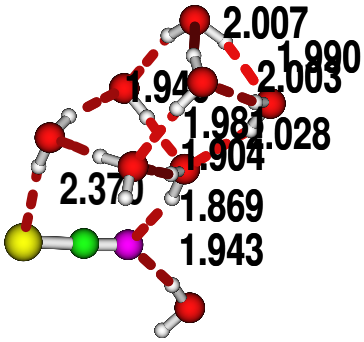
(n)Isomer 14



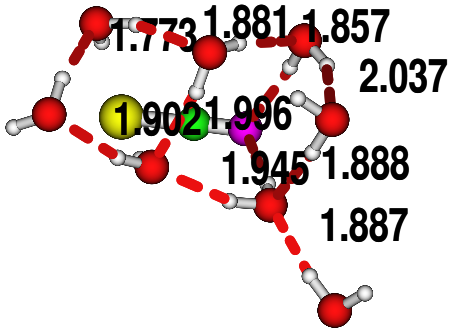
(o)Isomer 15



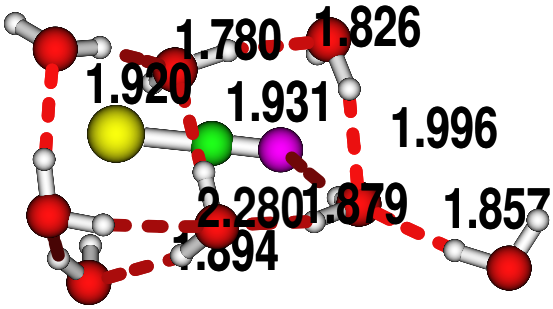
(p)Isomer 16



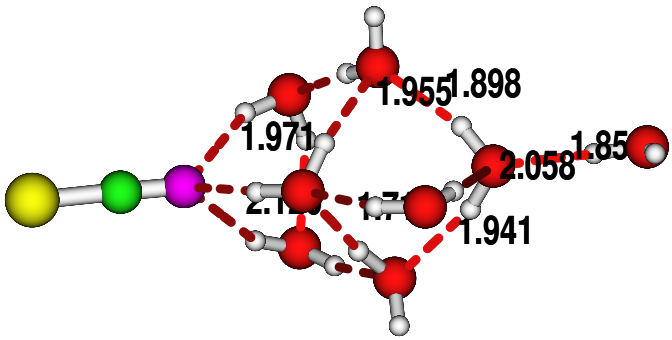
(q)Isomer 17



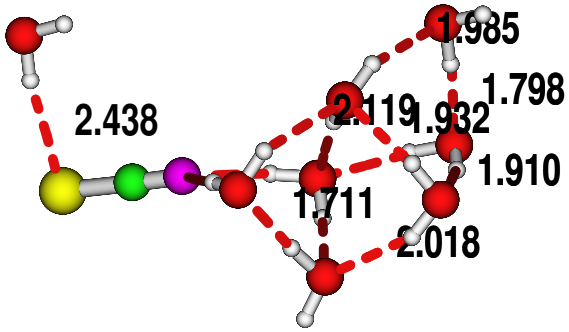
(r)Isomer 18



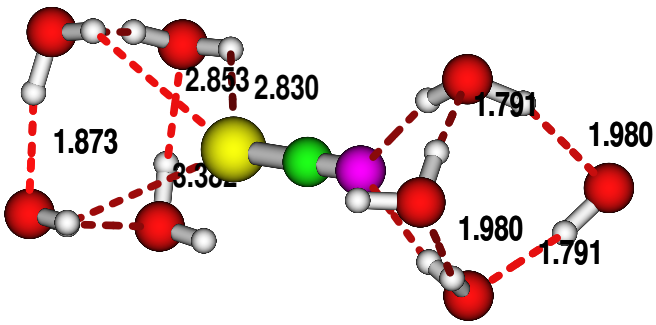
(s)Isomer 19



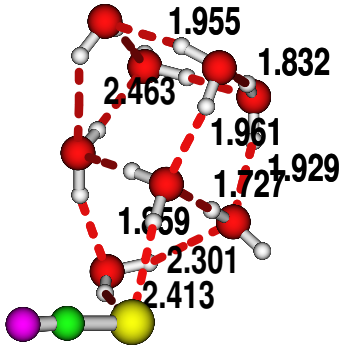
(t)Isomer 20



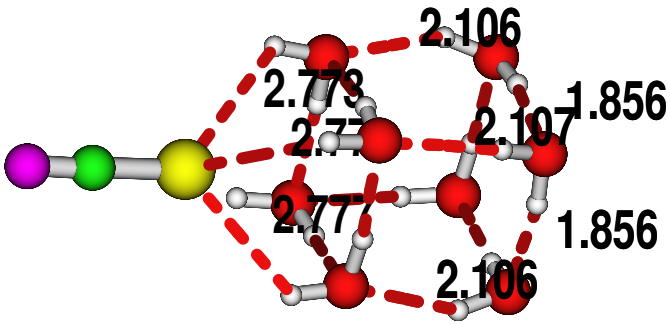
(u)Isomer 21



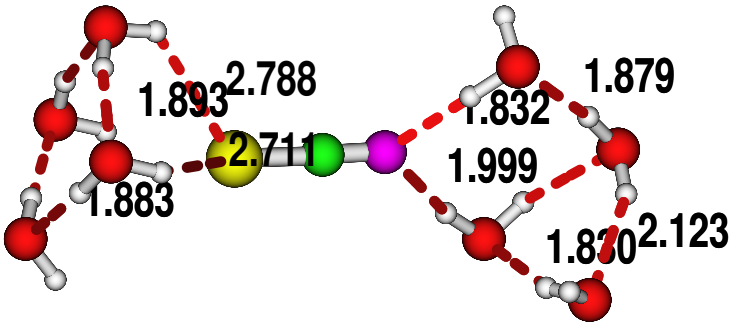
(v)Isomer 22



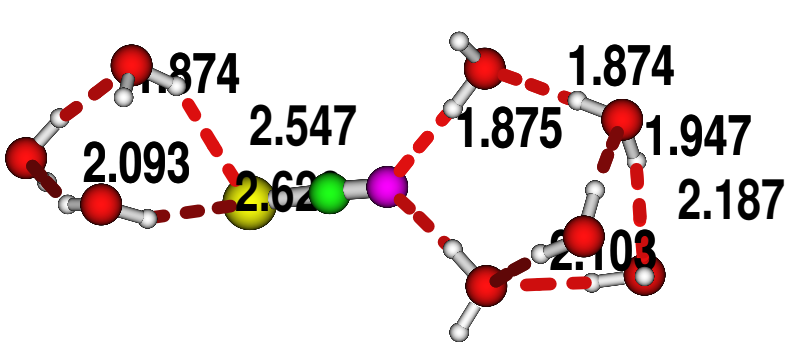
(w)Isomer 23



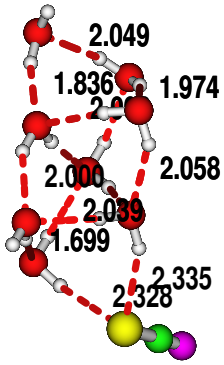
(x)Isomer 24



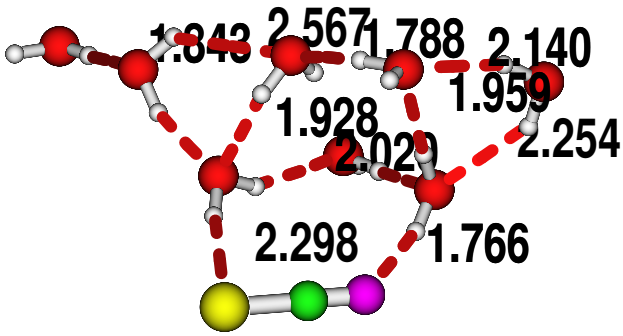
(y)Isomer 25



(z)Isomer 26

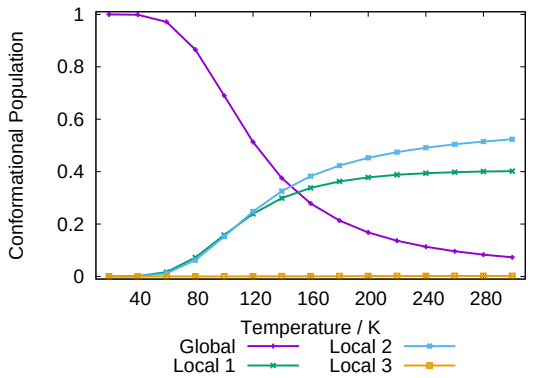


(aa)Isomer 27

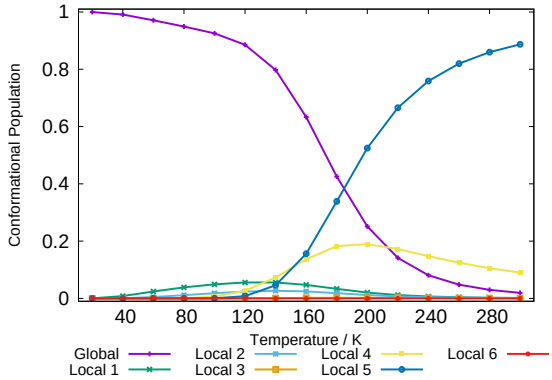


(bb)Isomer 28

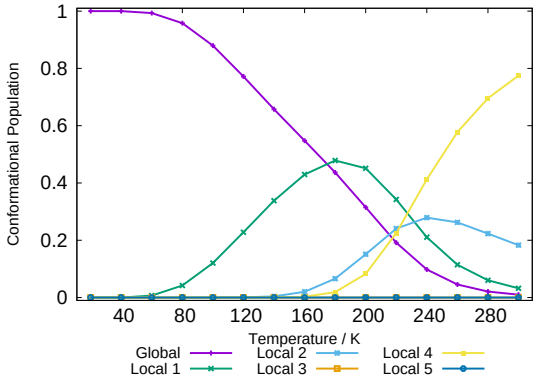
FIG. 8. Optimized structure of $SCN^{(-)}(H_2O)_8$ at DFT(B3LYP)/6-311++G(3df,3pd). For ease of visualization, S atoms are shown in yellow, C atoms are shown in green, N atoms are shown in pink and O and H atoms are shown in red and gray respectively.



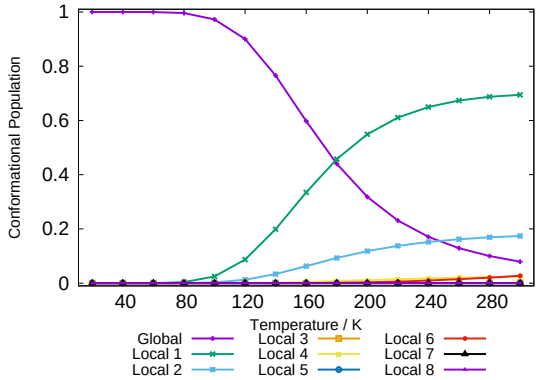
(a)for $SCN^{(-)}(H_2O)_2$



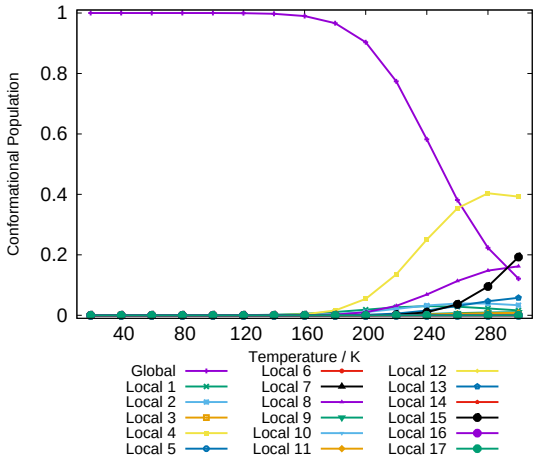
(b)for $SCN^{(-)}(H_2O)_3$



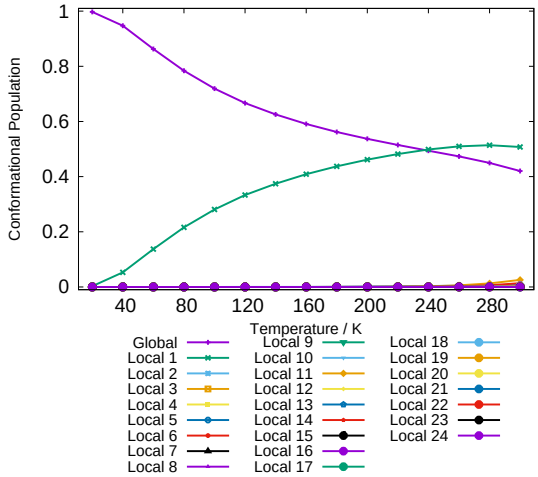
(c)for $SCN^{(-)}(H_2O)_4$



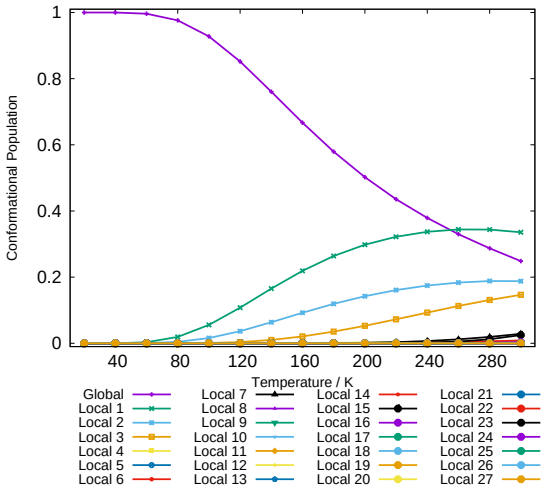
(d)for $SCN^{(-)}(H_2O)_5$



(e)for $SCN^{(-)}(H_2O)_6$



(f)for $SCN^{(-)}(H_2O)_7$



(g)for $SCN^{(-)}(H_2O)_8$

FIG. 9. Variations in conformational populations with temperature at $DFT(B3LYP)/6-311++G(3df,3pd)$ level of theory.

TABLES

TABLE I. Energies (in kCal/mol) of different isomers of $SCN^{(-)}(H_2O)_n$ system calculated at different levels of theory. [a = DFT(B3LYP)/6-311++G(3df,3pd), b = DFT(B3LYP)/6-311++G(3df,3pd) with BSSE correction, c = DFT(wB97xD)/6-311++G(3df,3pd), d = DFT(wB97xD)/6-311++G(3df,3pd) with BSSE correction, e = DFT(B3LYP)/6-31+G(d,p), f = DFT(B3LYP)/6-31+G(d,p) with BSSE correction]

Fig.	a	b	c	d	e	f
1(a)	-356215.50780	-356215.20492	-356160.29636	-356159.98373	-356158.92111	-356158.19034
2(a)	-404208.77682	-404208.17491	-404138.50057	-404137.83117	-404134.30777	-404132.76664
2(b)	-404207.33336	-404206.90079	-404136.40355	-404135.93499	-404132.50471	-404131.27596
2(c)	-404207.20085	-404206.68322	-404136.97180	-404136.42465	-404132.04476	-404130.98155
2(d)	-404207.16590	-404206.51738	-404138.18978	-404137.46916	-404132.39427	-404131.11817
3(a)	-452202.35914	-452201.29020	-452118.52470	-452117.35231	-452110.00829	-452107.36077
3(b)	-452202.34692	-452201.15029	-452119.21930	-452117.91755	-452109.61266	-452107.17762
3(c)	-452202.13427	-452200.89968	-452119.00457	-452117.66154	-452109.31201	-452106.95643
3(d)	-452200.33574	-452199.21297	-452119.00414	-452117.66115	-452107.46527	-452105.08211
3(e)	-452199.31122	-452198.38899	-452114.40640	-452113.40055	-452105.97751	-452104.14078
3(f)	-452197.44636	-452196.72898	-452119.00473	-452117.66236	-452104.06104	-452102.38040
3(g)	-452197.09937	-452195.92577	-452113.16079	-452111.89995	-452104.53294	-452102.20828
4(a)	-500197.70837	-500195.91155	-500100.00515	-500098.05844	-500087.39461	-500083.49605
4(b)	-500196.51585	-500194.80167	-500096.90168	-500095.08641	-500086.54500	-500082.49055
4(c)	-500192.47504	-500191.20042	-500095.21631	-500093.50784	-500081.40358	-500078.46637
4(d)	-500191.59682	-500189.88175	-500093.02391	-500091.13207	-500081.47316	-500077.85082
4(e)	-500189.17107	-500188.00228	-500097.46856	-500095.58801	-500077.25362	-500075.01359
4(f)	-500187.42215	-500185.92865	-500094.29471	-500092.58501	-500079.09077	-500073.57109
5(a)	-548191.02790	-548188.74095	-548077.58012	-548075.06582	-548063.20831	-548057.80059
5(b)	-548188.74683	-548186.68690	-548075.07475	-548072.82954	-548060.08112	-548055.48005
5(c)	-548188.50968	-548186.50175	-548072.59290	-548070.36009	-548060.72970	-548055.72474
5(d)	-548188.25224	-548186.00391	-548075.45550	-548072.94402	-548060.46543	-548055.44417
5(e)	-548188.05523	-548185.95434	-548072.64309	-548070.25975	-548060.90036	-548055.71034
5(f)	-548186.64203	-548184.42091	-548073.48001	-548070.98475	-548058.84362	-548053.86734

5(g)	-548186.07492	-548184.08851	-548071.76402	-548069.54196	-548057.37626	-548053.09921
5(h)	-548182.13927	-548179.93381	-548067.68129	-548065.22393	-548054.47474	-548049.56804
6(a)	-596185.86781	-596182.98018	-596043.92127	-596054.06995	-596026.49753	-596033.62701
6(b)	-596183.42555	-596180.63821	-596054.01434	-596050.94700	-596037.79631	-596031.08457
6(c)	-596181.85148	-596179.20720	-596054.16681	-596051.25148	-596035.24689	-596029.35020
6(d)	-596180.60765	-596177.96143	-596052.38746	-596049.45749	-596034.56763	-596028.52402
6(e)	-596180.52590	-596178.04084	-596051.60160	-596048.81077	-596034.13135	-596028.20454
6(f)	-596180.22861	-596177.59145	-596050.46925	-596047.48313	-596035.42971	-596028.98040
6(g)	-596179.57638	-596176.92585	-596052.02286	-596048.90908	-596034.15748	-596027.80462
6(h)	-596179.50643	-596176.81009	-596053.90257	-596050.80249	-596033.52971	-596027.68026
6(i)	-596179.47378	-596177.05073	-596053.90257	-596047.51089	-596033.52971	-596027.43339
6(j)	-596179.41366	-596177.01019	-596048.78316	-596046.10346	-596033.15662	-596027.50636
6(k)	-596179.18682	-596176.65156	-596050.79653	-596047.93336	-596033.20752	-596027.48282
6(l)	-596179.04034	-596176.55390	-596050.80089	-596048.09867	-596032.09509	-596026.82333
6(m)	-596178.96561	-596176.25105	-596052.02286	-596048.13908	-596034.15748	-596027.36875
6(n)	-596178.10825	-596175.79297	-596049.08651	-596046.23409	-596032.23428	-596026.74209
6(o)	-596174.31631	-596172.08049	-596045.49182	-596043.07149	-596027.23821	-596022.47163
6(p)	-596173.36983	-596171.31141	-596049.84255	-596047.08757	-596025.14700	-596020.76417
6(q)	-596172.14362	-596169.50602	-596043.92127	-596040.98812	-596026.49753	-596020.86987
6(r)	-596168.58556	-596166.23616	-596045.81490	-596042.77658	-596022.52562	-596016.89319
7(a)	-644179.98069	-644176.54502	-644032.14138	-644031.23948	-644012.60290	-644009.53439
7(b)	-644179.57265	-644176.21117	-644034.55224	-644030.79236	-644016.98560	-644008.88677
7(c)	-644177.01977	-644173.67340	-644032.46651	-644028.72662	-644014.19877	-644006.13706
7(d)	-644175.05353	-644171.61906	-644032.14138	-644028.29304	-644012.60290	-644004.43663
7(e)	-644175.04639	-644171.69536	-644031.07037	-644027.36641	-644012.16276	-644004.48832
7(f)	-644175.02288	-644171.66849	-644031.12322	-644027.40536	-644012.15083	-644004.48036
7(g)	-644174.34714	-644171.06141	-644029.71961	-644026.06355	-644011.61549	-644003.95639
7(h)	-644174.16277	-644170.86766	-644032.14134	-644028.29318	-644012.60248	-644003.29840
7(i)	-644174.11158	-644170.91031	-644029.85465	-644026.29461	-644011.67644	-644003.68723
7(j)	-644173.65825	-644170.28733	-644031.04458	-644027.29294	-644010.33119	-644002.83252

7(k)	-644173.64194	-644170.53016	-644030.86074	-644027.42416	-644009.85336	-644002.55070
7(l)	-644173.11392	-644170.05713	-644028.37099	-644024.96463	-644009.28368	-644001.94765
7(m)	-644172.91723	-644169.84806	-644028.72450	-644025.29963	-644008.64390	-644001.77917
7(n)	-644172.34011	-644169.30505	-644030.45124	-644027.11846	-644007.49272	-644001.07989
7(o)	-644172.21209	-644169.23236	-644028.04814	-644024.75720	-644008.10165	-644001.03566
7(p)	-644172.14775	-644169.07336	-644030.35117	-644026.98164	-644007.34973	-644000.78899
7(q)	-644171.67899	-644168.70000	-644029.50651	-644026.11852	-644007.43489	-644000.42393
7(r)	-644171.12539	-644168.08345	-644026.72326	-644023.26952	-644007.81888	-644000.73842
7(s)	-644171.00007	-644168.03373	-644026.84926	-644023.56765	-644007.14831	-644000.05847
7(t)	-644170.01188	-644167.16728	-644026.72301	-644023.27078	-644006.47494	-643999.71572
7(u)	-644168.59802	-644165.72535	-644025.96783	-644022.59719	-644005.77582	-643998.23799
7(v)	-644168.56810	-644165.68815	-644023.65826	-644020.55464	-644003.94533	-643997.71918
7(w)	-644167.99533	-644165.16598	-644024.38385	-644021.33107	-644003.44637	-643997.18854
7(x)	-644167.02376	-644163.75396	-644024.71353	-644021.06995	-644005.65979	-643997.05757
7(y)	-644159.36221	-644156.64277	-644020.28362	-644016.83550	-643995.91402	-643989.16716
8(a)	-692173.42391	-692169.45841	-692013.61798	-692009.18451	-691993.29762	-691983.61824
8(b)	-692172.58624	-692168.71251	-692013.42634	-692009.08427	-691992.00009	-691982.80891
8(c)	-692172.44862	-692168.55144	-692013.27415	-692008.92873	-691991.95035	-691982.65661
8(d)	-692171.43073	-692167.62095	-692012.08047	-692007.81562	-691990.28868	-691981.38425
8(e)	-692171.30895	-692167.31322	-692011.57442	-692007.14352	-691990.77723	-691981.52807
8(f)	-692170.06519	-692166.04028	-692013.84253	-692009.32809	-691989.74210	-691980.26036
8(g)	-692169.40365	-692165.53128	-692009.97505	-692005.63897	-691989.65787	-691979.52514
8(h)	-692168.68719	-692164.94162	-692009.70035	-692005.48731	-691987.57089	-691978.60643
8(i)	-692167.57889	-692163.82340	-692010.70819	-692006.51176	-691986.68721	-691977.79456
8(j)	-692167.50768	-692163.82357	-692008.33327	-692004.21727	-691986.57872	-691977.59310
8(k)	-692167.26802	-692163.49573	-692009.32449	-692005.03839	-691987.92477	-691977.41333
8(l)	-692167.24273	-692163.55475	-692010.55217	-692006.38691	-691986.57782	-691977.86433
8(m)	-692167.09916	-692163.38494	-692007.65146	-692003.48587	-691986.29238	-691977.28339
8(n)	-692166.88776	-692163.15187	-692008.69534	-692004.48154	-691986.67009	-691977.36168
8(o)	-692166.77265	-692162.97902	-692008.78964	-692004.56687	-691985.50138	-691976.83876

8(p)	-692166.10593	-692162.50256	-692009.65490	-692005.65826	-691983.91696	-691975.76569
8(q)	-692165.63863	-692162.06902	-692010.44812	-692006.17246	-691984.36462	-691976.12640
8(r)	-692165.63074	-692161.97413	-692008.43071	-692004.33651	-691983.96842	-691975.48851
8(s)	-692165.36507	-692161.75342	-692006.82776	-692002.81211	-691983.70830	-691975.40621
8(t)	-692164.51378	-692160.95349	-692004.42666	-692000.45258	-691984.28773	-691975.25652
8(u)	-692163.46222	-692160.02664	-692004.44870	-692000.56627	-691982.64370	-691974.31496
8(v)	-692162.25364	-692158.78399	-692002.55381	-691998.82657	-691980.19539	-691972.47306
8(w)	-692161.58277	-692157.71822	-692002.99416	-691998.66059	-691981.84205	-691972.47071
8(x)	-692161.44001	-692157.48373	-692003.93890	-691999.49777	-691981.44256	-691972.33087
8(y)	-692161.18085	-692157.82402	-692001.43087	-691997.76213	-691978.67607	-691971.23857
8(z)	-692159.54684	-692156.44812	-692005.09334	-692001.25480	-691976.68587	-691969.70031
8(aa)	-692159.43647	-692155.71446	-692001.84862	-691997.61425	-691979.47881	-691970.62224
8(bb)	-692159.26674	-692156.04761	-692000.73329	-691996.98055	-691978.58635	-691969.98757

TABLE II. Relative Energies (in kCal/mol) of different isomers of $SCN^{(-)}(H_2O)_n$ system calculated at different levels of theory. [a = DFT(B3LYP)/6-311++G(3df,3pd), b = DFT(B3LYP)/6-311++G(3df,3pd) with BSSE correction, c = DFT(wB97xD)/6-311++G(3df,3pd), d = DFT(wB97xD)/6-311++G(3df,3pd) with BSSE correction, e = DFT(B3LYP)/6-31+G(d,p), f = DFT(B3LYP)/6-31+G(d,p) with BSSE correction]

Fig.	a	b	c	d	e	f
1(a)	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000
2(a)	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000
2(b)	1.443468509	1.274121025	2.097017883	1.896182951	1.803061007	1.490685351
2(c)	1.575977830	1.491691953	1.528764008	1.406522451	2.263006725	1.785089587
2(d)	1.610928233	1.657526653	0.310786684	0.362016025	1.913496423	1.648473956
3(a)	0.000000000	0.000000000	0.694596660	0.565237752	0.000000000	0.000000000
3(b)	0.012223887	0.139903880	0.000000000	0.000000000	0.395625983	0.183149708
3(c)	0.224876226	0.390516259	0.214733788	0.256002956	0.696278386	0.404342321
3(d)	2.023405359	2.077226553	0.215160494	0.256399911	2.543020337	2.278656465
3(e)	3.047920843	2.901212109	4.812904567	4.516998601	4.030776592	3.219982970
3(f)	4.912782134	4.561217104	0.214570635	0.255186673	5.947247411	4.980364592
3(g)	5.259770474	5.364432649	6.058511139	6.017600474	5.475347635	5.152492275
4(a)	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000
4(b)	1.192519259	1.109875112	3.103461718	2.972029865	0.849604084	1.005496658
4(c)	5.233330984	4.711124179	4.788833299	4.550605170	5.991022481	5.029675609
4(d)	6.111555781	6.029794216	6.981238917	6.926375504	5.921450491	5.645227257
4(e)	8.537297710	7.909268849	2.536588364	2.470432184	10.140988247	8.482456116
4(f)	10.286224719	9.982896973	5.710437835	5.473431130	8.303840918	9.924955276
5(a)	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000	0.000000000
5(b)	2.281067079	2.054049419	2.505369761	2.236274037	3.127181581	2.320543654
5(c)	2.518221785	2.239202954	4.987220461	4.705724369	2.478606476	2.075853577
5(d)	2.775656974	2.737035057	2.124622031	2.121799132	2.742875872	2.356420835
5(e)	2.972671146	2.786612713	4.937025968	4.806066283	2.307948963	2.090248755
5(f)	4.385871101	4.320036398	4.100110128	4.081063236	4.364680729	3.933253686

5(g)	4.952982909	4.652438916	5.816104178	5.523860024	5.832042922	4.701377231
5(h)	8.888625907	8.807138975	9.898826015	9.841891066	8.733565773	8.232546593
6(a)	0.000000000	0.000000000	10.245537623	0.000000000	11.298787400	0.000000000
6(b)	2.442261747	2.341967189	0.152466009	3.122947704	0.000000000	2.542438174
6(c)	4.016325673	3.772976961	0.000000000	2.818469612	2.549420935	4.276809580
6(d)	5.260153255	5.018744017	1.779347419	4.612460136	3.228687536	5.102993467
6(e)	5.341905207	4.939341575	2.565209077	5.259173098	3.664963591	5.422471007
6(f)	5.639196669	5.388730535	3.697556440	6.586819921	2.366608561	4.646605319
6(g)	6.291425135	6.054325927	2.143949327	5.160866312	3.638834091	5.822384983
6(h)	6.361372376	6.170088232	0.264244296	3.267457294	4.266607253	5.946748063
6(i)	6.394028604	5.929451761	0.264244296	6.559059155	4.266607253	6.193614204
6(j)	6.454143397	5.969983800	5.383649656	7.966489028	4.639693090	6.120650793
6(k)	6.680985610	6.328614353	3.370278804	6.136589618	4.588795786	6.144188874
6(l)	6.827467060	6.426273050	3.365923887	5.971271387	5.701225994	6.803683570
6(m)	6.902201572	6.729127440	2.143949327	5.930863004	3.638834091	6.258256049
6(n)	7.759557909	7.187209466	5.080298961	7.835855195	5.562031812	6.884914628
6(o)	11.551496187	10.899687769	8.674994026	10.998453397	10.558100159	11.155383243
6(p)	12.497978969	11.668765157	4.324256560	6.982372176	12.649319853	12.862841933
6(q)	13.724184826	13.474155105	10.245537623	13.081826600	11.298787400	12.757139907
6(r)	17.282247762	16.744021021	8.351914429	11.293364919	15.270691040	16.733815100
7(a)	0.000000000	0.000000000	2.410866814	0.000000000	4.382696530	0.000000000
7(b)	0.408038123	0.333851702	0.000000000	0.447127138	0.000000000	0.647623292
7(c)	2.960916636	2.871623574	2.085728985	2.512859904	2.786826645	3.397328570
7(d)	4.927161517	4.925964839	2.410866814	2.946441211	4.382696530	5.097755626
7(e)	4.934302576	4.849665502	3.481868837	3.873075334	4.822844319	5.046069830
7(f)	4.957809086	4.876533992	3.429019978	3.834127838	4.834767002	5.054029202
7(g)	5.633549082	5.483609436	4.832633469	5.175936332	5.370107999	5.577999730
7(h)	5.817917680	5.677361513	2.410904464	2.946299656	4.383123237	6.235990305
7(i)	5.869103639	5.634712557	4.697593402	4.944872739	5.309157990	5.847155358
7(j)	6.322441680	6.257692863	3.507665757	3.946541446	6.654406813	6.701870750

7(k)	6.338744380	6.014858052	3.691507247	3.815323800	7.132236554	6.983688300
7(l)	6.866768615	6.487895434	6.181252018	6.274857752	7.701921152	7.586738230
7(m)	7.063455226	6.696966182	5.827738206	5.939854904	8.341698573	7.755216773
7(n)	7.640582088	7.239974556	4.101007467	4.121018725	9.492883774	8.454496832
7(o)	7.768594048	7.312660149	6.504105712	6.482282630	8.883954725	8.498728933
7(p)	7.832938883	7.471661254	4.201070149	4.257844218	9.635868113	8.745397303
7(q)	8.301694835	7.845018309	5.045735732	5.120967889	9.550715059	9.110460833
7(r)	8.855296362	8.461571910	7.828979297	7.969967899	9.166723105	8.795968532
7(s)	8.980622581	8.511287819	7.702987918	7.671835696	9.837292422	9.475917083
7(t)	9.968805886	9.377741680	7.829236576	7.968707154	10.510660432	9.818671852
7(u)	11.382666609	10.819668917	8.584413014	8.642297091	11.209781437	11.296398099
7(v)	11.412592542	10.856873343	10.893987227	10.684844561	13.040270889	11.815214126
7(w)	11.985358212	11.379040169	10.168397867	9.908413081	13.539235154	12.345849761
7(x)	12.956931338	12.791061337	9.838710594	10.169529047	11.325814239	12.476822335
7(y)	20.618478522	19.902247579	14.268620947	14.403982349	21.071584385	20.367233654
8(a)	0.000000000	0.000000000	0.224554313	0.143574267	0.000000000	0.000000000
8(b)	0.837668851	0.745899770	0.416195748	0.243818696	1.297532992	0.809326374
8(c)	0.975287983	0.906973095	0.568385653	0.399359264	1.347275679	0.961622385
8(d)	1.993177593	1.837457350	1.762059530	1.512470657	3.008946221	2.233986451
8(e)	2.114964658	2.145186795	2.268114653	2.184566710	2.520398616	2.090171196
8(f)	3.358720077	3.418131603	0.000000000	0.000000000	3.555525915	3.357876181
8(g)	4.020259531	3.927134311	3.867479767	3.689119835	3.639756530	4.093100748
8(h)	4.736718626	4.516790292	4.142184648	3.840776757	5.726734259	5.011802298
8(i)	5.845019820	5.635011866	3.134341466	2.816328169	6.610412114	5.823679281
8(j)	5.916229611	5.634845654	5.509264529	5.110813022	6.718908526	6.025135346
8(k)	6.155888080	5.962676217	4.518044077	4.289699385	5.372856491	6.204909527
8(l)	6.181182992	5.903656810	3.290365455	2.941173175	6.719805864	5.753909666
8(m)	6.324750916	6.073472435	6.191072544	5.842215625	7.005247435	6.334846600
8(n)	6.536152627	6.306542235	5.147197761	4.846548879	6.627530577	6.256561109
8(o)	6.651262990	6.479391516	5.052889342	4.761213068	7.796242121	6.779473759

8(p)	7.317985673	6.955855719	4.187628893	3.669821776	9.380666231	7.852542938
8(q)	7.785279528	7.389392491	3.394412823	3.155628400	8.933007152	7.491833252
8(r)	7.793173599	7.484283403	5.411824838	4.991578370	9.329204168	8.129725327
8(s)	8.058842342	7.704991883	7.014773031	6.515974171	9.589325726	8.212022900
8(t)	8.910134426	8.504919869	9.415869520	8.875509889	9.009895904	8.361718084
8(u)	9.961696202	9.431769462	9.393831383	8.761813174	10.653920876	9.303281027
8(v)	11.170267157	10.674416848	11.288722146	10.501519005	13.102231188	11.145173310
8(w)	11.841137679	11.740187599	10.848373553	10.667493147	11.455570676	11.147531288
8(x)	11.983902390	11.974682866	9.903632738	9.830316328	11.855068392	11.287363441
8(y)	12.243057583	11.634395509	12.411663140	11.565954895	14.621551176	12.379668899
8(z)	13.877067502	13.010294711	8.749190762	8.073283569	16.611754374	13.917931013
8(aa)	13.987440167	13.743950928	11.993917443	11.713838284	13.818815785	12.995997752
8(bb)	14.157175241	13.410804873	13.109246746	12.347539343	14.711272500	13.630664077

TABLE III. Relative Stability of different isomers of $SCN^{(-)}(H_2O)_n$ system at different levels of theory. [a = DFT(B3LYP)/6-311++G(3df,3pd), b = DFT(B3LYP)/6-311++G(3df,3pd) with BSSE correction, c = DFT(wB97xD)/6-311++G(3df,3pd), d = DFT(wB97xD)/6-311++G(3df,3pd) with BSSE correction, e = DFT(B3LYP)/6-31+G(d,p), f = DFT(B3LYP)/6-31+G(d,p) with BSSE correction]

Fig.	a	b	c	d	e	f
1(a)	Global	Global	Global	Global	Global	Global
2(a)	Global	Global	Global	Global	Global	Global
2(b)	Local 1	Local 1	Local 3	Local 3	Local 1	Local 1
2(c)	Local 2	Local 2	Local 2	Local 2	Local 3	Local 3
2(d)	Local 3	Local 3	Local 1	Local 1	Local 2	Local 2
3(a)	Global	Global	Local 4	Local 4	Global	Global
3(b)	Local 1	Local 1	Global	Global	Local 1	Local 1
3(c)	Local 2	Local 2	Local 2	Local 2	Local 2	Local 2
3(d)	Local 3	Local 3	Local 3	Local 3	Local 3	Local 3
3(e)	Local 4	Local 4	Local 5	Local 5	Local 4	Local 4
3(f)	Local 5	Local 5	Local 1	Local 1	Local 6	Local 5
3(g)	Local 6	Local 6	Local 6	Local 6	Local 5	Local 6
4(a)	Global	Global	Global	Global	Global	Global
4(b)	Local 1	Local 1	Local 2	Local 2	Local 1	Local 1
4(c)	Local 2	Local 2	Local 3	Local 3	Local 3	Local 2
4(d)	Local 3	Local 3	Local 5	Local 5	Local 2	Local 3
4(e)	Local 4	Local 4	Local 1	Local 1	Local 5	Local 4
4(f)	Local 5	Local 5	Local 4	Local 4	Local 4	Local 5
5(a)	Global	Global	Global	Global	Global	Global
5(b)	Local 1	Local 1	Local 2	Local 2	Local 4	Local 3
5(c)	Local 2	Local 2	Local 5	Local 4	Local 2	Local 1
5(d)	Local 3	Local 3	Local 1	Local 1	Local 3	Local 4
5(e)	Local 4	Local 4	Local 4	Local 5	Local 1	Local 2
5(f)	Local 5	Local 5	Local 3	Local 3	Local 5	Local 5

5(g)	Local 6	Local 6	Local 6	Local 6	Local 6	Local 6
5(h)	Local 7	Local 7	Local 7	Local 7	Local 7	Local 7
6(a)	Global	Global	Local 16	Global	Local 14	Global
6(b)	Local 1	Local 1	Local 1	Local 2	Global	Local 1
6(c)	Local 2	Local 2	Global	Local 1	Local 2	Local 2
6(d)	Local 3	Local 4	Local 4	Local 4	Local 3	Local 4
6(e)	Local 4	Local 3	Local 7	Local 6	Local 6	Local 5
6(f)	Local 5	Local 5	Local 10	Local 11	Local 1	Local 3
6(g)	Local 6	Local 8	Local 6	Local 5	Local 5	Local 6
6(h)	Local 7	Local 9	Local 3	Local 3	Local 8	Local 7
6(i)	Local 8	Local 6	Local 2	Local 10	Local 7	Local 10
6(j)	Local 9	Local 7	Local 13	Local 14	Local 10	Local 8
6(k)	Local 10	Local 10	Local 9	Local 9	Local 9	Local 9
6(l)	Local 11	Local 11	Local 8	Local 8	Local 12	Local 12
6(m)	Local 12	Local 12	Local 5	Local 7	Local 4	Local 11
6(n)	Local 13	Local 13	Local 12	Local 13	Local 11	Local 13
6(o)	Local 14	Local 14	Local 15	Local 15	Local 13	Local 14
6(p)	Local 15	Local 15	Local 11	Local 12	Local 16	Local 16
6(q)	Local 16	Local 16	Local 17	Local 17	Local 15	Local 15
6(r)	Local 17	Local 17	Local 14	Local 16	Local 17	Local 17
7(a)	Global	Global	Local 2	Global	Local 2	Global
7(b)	Local 1	Local 1	Global	Local 1	Global	Local 1
7(c)	Local 2	Local 2	Local 1	Local 2	Local 1	Local 2
7(d)	Local 3	Local 5	Local 3	Local 4	Local 3	Local 5
7(e)	Local 4	Local 3	Local 6	Local 7	Local 5	Local 3
7(f)	Local 5	Local 4	Local 5	Local 6	Local 6	Local 4
7(g)	Local 6	Local 6	Local 12	Local 13	Local 8	Local 6
7(h)	Local 7	Local 8	Local 4	Local 3	Local 4	Local 8
7(i)	Local 8	Local 7	Local 11	Local 11	Local 7	Local 7
7(j)	Local 9	Local 10	Local 7	Local 8	Local 9	Local 9

7(k)	Local 10	Local 9	Local 8	Local 5	Local 10	Local 10
7(l)	Local 11	Local 11	Local 15	Local 15	Local 11	Local 11
7(m)	Local 12	Local 12	Local 14	Local 14	Local 12	Local 12
7(n)	Local 13	Local 13	Local 9	Local 9	Local 15	Local 13
7(o)	Local 14	Local 14	Local 16	Local 16	Local 13	Local 14
7(p)	Local 15	Local 15	Local 10	Local 10	Local 17	Local 15
7(q)	Local 16	Local 16	Local 13	Local 12	Local 16	Local 17
7(r)	Local 17	Local 17	Local 18	Local 19	Local 14	Local 16
7(s)	Local 18	Local 18	Local 17	Local 17	Local 18	Local 18
7(t)	Local 19	Local 19	Local 19	Local 18	Local 19	Local 19
7(u)	Local 20	Local 20	Local 20	Local 20	Local 20	Local 20
7(v)	Local 21	Local 21	Local 23	Local 23	Local 22	Local 21
7(w)	Local 22	Local 22	Local 22	Local 21	Local 23	Local 22
7(x)	Local 23	Local 23	Local 21	Local 22	Local 21	Local 23
7(y)	Local 24	Local 24	Local 24	Local 24	Local 24	Local 24
8(a)	Global	Global	Local 1	Local 1	Global	Global
8(b)	Local 1	Local 1	Local 2	Local 2	Local 1	Local 1
8(c)	Local 2	Local 2	Local 3	Local 3	Local 2	Local 2
8(d)	Local 3	Local 3	Local 4	Local 4	Local 4	Local 4
8(e)	Local 4	Local 4	Local 5	Local 5	Local 3	Local 3
8(f)	Local 5	Local 5	Global	Global	Local 5	Local 5
8(g)	Local 6	Local 6	Local 9	Local 10	Local 6	Local 6
8(h)	Local 7	Local 7	Local 10	Local 11	Local 8	Local 7
8(i)	Local 8	Local 9	Local 6	Local 6	Local 9	Local 9
8(j)	Local 9	Local 8	Local 16	Local 16	Local 11	Local 10
8(k)	Local 10	Local 11	Local 12	Local 12	Local 7	Local 11
8(l)	Local 11	Local 10	Local 7	Local 7	Local 12	Local 8
8(m)	Local 12	Local 12	Local 17	Local 17	Local 13	Local 13
8(n)	Local 13	Local 13	Local 14	Local 14	Local 10	Local 12
8(o)	Local 14	Local 14	Local 13	Local 13	Local 14	Local 14

8(p)	Local 15	Local 15	Local 11	Local 9	Local 18	Local 16
8(q)	Local 16	Local 16	Local 8	Local 8	Local 15	Local 15
8(r)	Local 17	Local 17	Local 15	Local 15	Local 17	Local 17
8(s)	Local 18	Local 18	Local 18	Local 18	Local 19	Local 18
8(t)	Local 19	Local 19	Local 21	Local 21	Local 16	Local 19
8(u)	Local 20	Local 20	Local 20	Local 20	Local 20	Local 20
8(v)	Local 21	Local 21	Local 24	Local 23	Local 23	Local 21
8(w)	Local 22	Local 23	Local 23	Local 24	Local 21	Local 22
8(x)	Local 23	Local 24	Local 22	Local 22	Local 22	Local 23
8(y)	Local 24	Local 22	Local 26	Local 25	Local 25	Local 24
8(z)	Local 25	Local 25	Local 19	Local 19	Local 27	Local 27
8(aa)	Local 26	Local 27	Local 25	Local 26	Local 24	Local 25
8(bb)	Local 27	Local 26	Local 27	Local 27	Local 26	Local 26

TABLE IV. Charges on different atoms of the global minimum isomers of $SCN^{(-)}(H_2O)_n$ system obtained at DFT(B3LYP)/6-311++G(3df,3pd) level of theory using NBO analysis.

n =	1	2	3	4	5	6	7	8
S	-0.417	-0.376	-0.340	-0.396	-0.378	-0.347	-0.286	-0.354
C	0.106	0.121	0.126	0.077	0.089	0.102	0.142	0.118
N	-0.649	-0.695	-0.746	-0.634	-0.654	-0.669	-0.772	-0.664
O	-0.988	-0.989	-0.984	-0.986	-0.997	-0.990	-0.987	-0.988
H	0.510	0.508	0.494	0.479	0.496	0.495	0.489	0.492
H	0.439	0.447	0.476	0.493	0.501	0.486	0.497	0.484
O		-0.980	-0.984	-0.992	-0.982	-0.990	-0.987	-0.987
H		0.487	0.476	0.493	0.502	0.497	0.489	0.496
H		0.476	0.495	0.485	0.452	0.478	0.497	0.481
O			-0.984	-0.985	-0.993	-1.001	-0.996	-0.997
H			0.494	0.490	0.491	0.491	0.507	0.498
H			0.477	0.492	0.493	0.496	0.466	0.492
O				-0.990	-0.985	-0.997	-0.996	-0.995
H				0.478	0.478	0.497	0.497	0.464
H				0.495	0.498	0.485	0.489	0.506
O					-0.989	-0.980	-0.996	-1.006
H					0.477	0.482	0.497	0.464
H					0.499	0.491	0.489	0.508
O						-0.992	-1.006	-1.003
H						0.503	0.463	0.500
H						0.464	0.505	0.504
O							-1.002	-0.997
H							0.499	0.488
H							0.499	0.500
O								-0.989
H								0.498
H								0.486

TABLE V. Charges on different atoms of the global minimum isomers of $SCN^{(-)}(H_2O)_n$ system obtained at DFT(wB97xD)/6-311++G(3df,3pd) level of theory using NBO analysis.

n =	1	2	3	4	5	6	7	8
S	-0.438	-0.399	-0.661	-0.640	-0.397	-0.375	-0.295	-0.404
C	0.130	0.147	0.102	0.100	0.114	0.131	0.177	0.103
N	-0.656	-0.702	-0.399	-0.414	-0.661	-0.693	-0.791	-0.647
O	-0.987	-0.989	-0.990	-0.992	-0.987	-0.987	-0.989	-0.998
H	0.511	0.511	0.488	0.480	0.499	0.497	0.490	0.496
H	0.441	0.449	0.487	0.496	0.480	0.490	0.491	0.503
O		-0.979	-0.984	-0.994	-0.991	-1.001	-0.997	-1.007
H		0.486	0.493	0.494	0.478	0.484	0.497	0.502
H		0.476	0.481	0.486	0.500	0.501	0.485	0.500
O			-0.990	-0.986	-1.000	-0.985	-1.002	-1.008
H			0.486	0.492	0.502	0.494	0.495	0.502
H			0.485	0.492	0.496	0.480	0.490	0.495
O				-0.988	-0.994	-0.984	-0.998	-1.002
H				0.481	0.494	0.479	0.497	0.494
H				0.494	0.491	0.496	0.486	0.499
O					-0.982	-0.986	-0.992	-0.990
H					0.503	0.484	0.496	0.484
H					0.453	0.476	0.488	0.499
O						-0.975	-0.993	-0.992
H						0.502	0.508	0.498
H						0.472	0.471	0.488
O							-0.992	-0.991
H							0.508	0.498
H							0.470	0.486
O								-0.992
H								0.497
H								0.488

TABLE VI. Charges on different atoms of the global minimum isomers of $SCN^{(-)}(H_2O)_n$ system obtained at DFT(B3LYP)/6-31+G(d,p) level of theory using NBO analysis.

n =	1	2	3	4	5	6	7	8
S	-0.413	-0.371	-0.334	-0.383	-0.366	-0.365	-0.265	-0.635
C	0.088	0.105	0.111	0.059	0.072	0.071	0.127	0.103
N	-0.625	-0.669	-0.717	-0.606	-0.624	-0.610	-0.746	-0.340
O	-1.053	-1.047	-1.045	-1.049	-1.049	-1.056	-1.053	-1.047
H	0.476	0.514	0.518	0.508	0.526	0.531	0.510	0.509
H	0.528	0.506	0.507	0.521	0.505	0.518	0.529	0.520
O		-1.050	-1.045	-1.047	-1.047	-1.046	-1.048	-1.057
H		0.486	0.519	0.505	0.525	0.530	0.522	0.507
H		0.525	0.506	0.521	0.508	0.492	0.514	0.528
O			-1.045	-1.047	-1.051	-1.051	-1.047	-1.057
H			0.518	0.517	0.516	0.523	0.518	0.519
H			0.507	0.519	0.520	0.517	0.518	0.525
O				-1.050	-1.056	-1.055	-1.056	-1.064
H				0.511	0.520	0.510	0.523	0.526
H				0.519	0.529	0.533	0.514	0.530
O					-1.047	-1.046	-1.055	-1.058
H					0.492	0.494	0.529	0.517
H					0.528	0.531	0.510	0.527
O						-1.050	-1.060	-1.073
H						0.507	0.520	0.509
H						0.524	0.517	0.537
O							-1.056	-1.040
H							0.514	0.526
H							0.523	0.513
O								-1.047
H								0.524
H								0.507

TABLE VII. IR-frequencies [in cm^{-1}] of $SCN^{(-)}H_2O$ calculated at DFT $(B3LYP)/$ $6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
1(a)	3362.4,3877.3

TABLE VIII. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_2$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
2(a)	3320.1,3703.5,3759.4,3873.3
2(b)	3482.4,3504.0,3874.5,3875.0
2(c)	3420.1,3586.1,3858.8,3878.6
2(d)	3477.6,3649.4,3738.4,3858.5

TABLE IX. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_3$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
3(a)	3613.8,3620.2,3641.7,3731.0,3746.5,3749.2
3(b)	3601.4,3620.7,3649.5,3684.9,3693.6,3727.5
3(c)	3563.3,3602.0,3651.6,3678.9,3702.0,3709.4
3(d)	3439.1,3627.6,3690.1,3714.6,3750.7,3863.0
3(e)	3456.8,3505.5,3707.2,3761.0,3854.3,3878.9
3(f)	3576.4,3579.6,3599.6,3873.2,3873.5,3874.2
3(g)	3616.2,3662.3,3663.0,3710.8,3711.4,3728.4

TABLE X. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_4$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
4(a)	3496.3,3554.5,3584.5,3629.5,3657.0,3693.6,3699.9,3717.8
4(b)	3343.7,3360.2,3463.8,3484.9,3664.9,3665.5,3861.7,3862.0
4(c)	3599.0,3637.4,3656.2,3666.8,3729.3,3740.1,3744.8,3869.8
4(d)	3507.4,3566.7,3567.1,3596.9,3721.3,3727.3,3728.2,3744.7
4(e)	3495.2,3537.9,3648.0,3700.4,3791.7,3855.7,3862.9,3879.2
4(f)	3512.1,3579.7,3583.9,3613.4,3648.8,3743.3,3845.2,3881.3

TABLE XI. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_5$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
5(a)	3278.4,3466.6,3512.3,3549.3,3583.3,3600.6,3638.2,3719.6,3734.2,3873.8
5(b)	3483.9,3539.5,3541.1,3567.9,3592.0,3706.8,3719.7,3731.9,3746.7,3878.8
5(c)	3220.9,3362.3,3536.0,3595.4,3661.8,3708.7,3714.5,3737.9,3872.7,3876.3
5(d)	3390.2,3516.7,3530.1,3578.8,3616.5,3625.8,3644.7,3692.3,3711.9,3873.4
5(e)	3217.4,3227.4,3390.3,3424.2,3709.4,3712.5,3718.8,3767.5,3883.6,3883.6
5(f)	3219.5,3518.4,3562.2,3590.2,3610.0,3635.9,3706.4,3723.4,3783.2,3886.3
5(g)	3092.0,3569.6,3587.7,3635.1,3650.1,3687.2,3691.6,3715.3,3868.1,3878.3
5(h)	3065.5,3457.5,3513.4,3531.8,3557.1,3581.6,3714.8,3746.8,3869.7,3882.9

TABLE XII. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_6$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
6(a)	3267.7,3429.6,3492.6,3532.4,3554.1,3609.2,3661.6,3690.9,3704.9,3719.9,3727.0,3881.8
6(b)	3283.8,3298.4,3444.2,3504.0,3572.2,3591.8,3611.5,3629.9,3661.4,3680.6,3873.6,3874.8
6(c)	3480.6,3498.8,3556.4,3571.6,3598.4,3668.8,3669.2,3715.9,3727.8,3753.0,3757.4,3871.2
6(d)	3382.7,3524.6,3558.6,3593.0,3613.1,3643.0,3670.2,3682.4,3684.0,3732.3,3755.5,3874.3
6(e)	3347.9,3401.3,3489.7,3507.0,3557.8,3568.7,3579.8,3605.9,3812.9,3858.5,3863.4,3879.0
6(f)	3204.7,3246.6,3357.3,3395.9,3644.9,3679.9,3686.6,3721.2,3735.4,3794.8,3880.0,3885.7
6(g)	3310.8,3384.3,3500.6,3544.1,3547.8,3605.8,3640.3,3665.5,3690.5,3771.9,3860.5,3865.7
6(h)	3571.6,3577.3,3598.7,3616.6,3629.9,3649.1,3654.7,3666.0,3701.1,3712.3,3729.0,3762.7
6(i)	3431.0,3499.0,3558.3,3572.4,3610.2,3619.4,3638.0,3654.8,3696.9,3707.1,3880.3,3880.9
6(j)	3231.0,3353.1,3583.1,3623.4,3659.2,3701.4,3708.1,3719.6,3744.2,3773.1,3856.3,3880.4
6(k)	3353.7,3557.1,3589.2,3602.0,3641.9,3664.6,3674.3,3676.4,3710.1,3791.1,3796.6,3868.0
6(l)	3467.1,3533.4,3561.0,3575.2,3596.5,3702.9,3721.8,3733.6,3745.4,3765.3,3768.6,3862.2
6(m)	3207.2,3518.9,3558.9,3590.5,3597.5,3626.6,3653.5,3681.0,3697.7,3753.6,3796.8,3888.8
6(n)	3239.5,3256.2,3437.8,3470.8,3611.8,3703.2,3706.3,3718.2,3772.4,3867.2,3882.7,3882.9
6(o)	3595.6,3649.5,3653.1,3674.0,3679.1,3680.4,3732.2,3734.0,3736.6,3766.1,3767.5,3779.8
6(p)	3490.6,3602.8,3612.7,3631.8,3666.4,3668.7,3736.7,3751.8,3861.4,3867.8,3869.8,3871.3
6(q)	3575.3,3589.0,3632.3,3633.1,3645.5,3651.2,3697.4,3708.5,3724.4,3752.1,3753.1,3764.2
6(r)	3432.1,3490.7,3509.1,3548.6,3685.3,3696.0,3706.2,3752.5,3778.0,3794.2,3869.6,3873.3

TABLE XIII. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_7$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
7(a)	3108.0,3228.3,3451.3,3466.6,3518.6,3520.2,3586.8,3601.3,3669.2,3678.8,3696.1,3703.6, 3876.2,3888.0
7(b)	3270.6,3319.9,3440.5,3502.3,3530.4,3559.3,3608.7,3664.7,3689.7,3703.4,3718.4,3724.7, 3876.5,3878.8
7(c)	3163.9,3178.5,3428.0,3491.6,3589.7,3600.6,3614.3,3643.5,3650.6,3672.8,3691.2,3743.4, 3879.1,3880.1
7(d)	3103.0,3371.7,3532.4,3542.7,3560.7,3589.4,3602.5,3610.1,3628.3,3632.3,3711.0,3713.6, 3755.6,3889.0
7(e)	3196.7,3229.9,3328.3,3511.7,3578.8,3605.4,3625.9,3636.0,3642.7,3695.8,3702.5,3714.4, 3866.7,3879.8
7(f)	3119.7,3310.6,3371.5,3461.2,3557.4,3578.2,3634.6,3639.5,3677.3,3696.9,3700.1,3712.4, 3871.4,3876.7
7(g)	3193.2,3259.1,3352.4,3402.4,3576.5,3630.7,3636.7,3647.5,3685.3,3709.1,3718.6,3735.5, 3868.4,3880.4
7(h)	3091.9,3472.5,3475.8,3533.5,3540.6,3566.8,3595.0,3605.5,3652.5,3687.3,3712.4,3725.5, 3802.4,3887.1
7(i)	3161.1,3235.0,3404.1,3525.2,3602.9,3626.2,3639.4,3646.9,3676.5,3695.8,3721.1,3801.1, 3872.9,3883.2
7(j)	3268.4,3425.2,3529.9,3550.9,3565.2,3575.6,3622.3,3634.5,3644.0,3690.1,3702.2,3719.2, 3739.8,3876.6
7(k)	3416.2,3506.2,3533.9,3545.1,3572.3,3584.0,3599.2,3610.4,3646.0,3652.8,3714.4,3722.6, 3848.1,3880.8
7(l)	3269.1,3331.6,3430.8,3510.6,3556.6,3572.5,3609.5,3624.8,3659.9,3685.9,3721.4,3862.7, 3878.1,3880.2
7(m)	3430.0,3445.0,3493.7,3538.9,3582.1,3615.9,3627.5,3664.8,3688.1,3692.4,3703.6,3763.3, 3870.8,3871.0
7(n)	3460.6,3526.9,3549.3,3563.4,3585.2,3638.2,3658.9,3706.8,3720.9,3739.6,3757.4,3761.5,

	3769.2,3792.9
7(o)	3285.1,3447.1,3510.1,3534.1,3564.1,3584.0,3620.0,3640.2,3689.0,3740.9,3780.0,3824.3, 3867.0,3880.6
7(p)	3466.6,3533.2,3544.2,3576.9,3601.6,3646.1,3684.0,3721.4,3728.3,3734.9,3739.5,3768.6, 3771.8,3776.4
7(q)	3363.3,3469.4,3528.6,3580.1,3592.9,3597.6,3627.0,3631.6,3695.0,3740.9,3770.7,3810.7, 3865.5,3878.7
7(r)	3269.1,3301.9,3388.0,3408.0,3649.1,3687.6,3692.9,3700.3,3707.8,3739.5,3775.3,3797.3, 3879.4,3884.2
7(s)	3379.7,3439.1,3482.6,3502.4,3555.1,3563.3,3626.6,3666.6,3680.0,3691.0,3764.2,3850.0, 3875.1,3881.8
7(t)	3232.4,3275.6,3410.1,3443.7,3609.9,3645.2,3674.8,3689.5,3715.0,3736.1,3801.6,3869.7, 3879.4,3885.4
7(u)	3160.4,3277.8,3367.2,3461.0,3568.8,3634.0,3659.6,3682.4,3706.5,3750.9,3810.9,3855.7, 3870.3,3887.2
7(v)	3352.8,3381.3,3547.0,3569.2,3588.5,3637.1,3642.4,3644.7,3666.9,3733.8,3779.0,3796.6, 3866.5,3867.4
7(w)	3452.6,3524.7,3525.0,3557.7,3675.8,3684.1,3689.3,3734.7,3736.9,3739.1,3783.0,3786.2, 3786.6,3795.9
7(x)	3284.6,3382.6,3481.1,3533.9,3547.4,3560.5,3593.8,3610.0,3649.5,3705.0,3719.0,3749.4, 3865.2,3876.1
7(y)	3404.0,3431.8,3468.8,3546.3,3671.6,3697.2,3714.2,3720.2,3740.1,3748.3,3786.0,3811.5, 3870.9,3879.7

TABLE XIV. IR-frequencies [in cm^{-1}] of different isomers of $SCN^{(-)}(H_2O)_8$ calculated at DFT $(B3LYP)/\ 6-311++G(3df,3pd)$ level of theory.

Fig. No.	Peaks [in cm^{-1}]
8(a)	3026.4,3228.6,3425.7,3461.8,3490.2,3537.0,3545.4,3605.4,3628.2,3663.4,3667.1,3686.9, 3695.7,3708.7,3880.8,3883.6
8(b)	3111.8,3425.9,3472.1,3504.0,3528.7,3548.0,3573.9,3597.5,3624.9,3632.8,3656.2,3677.5, 3688.3,3712.4,3860.1,3885.5
8(c)	3082.1,3452.6,3465.1,3497.2,3533.7,3537.0,3574.0,3606.7,3620.5,3627.7,3649.3,3671.0, 3688.1,3703.1,3859.7,3887.4
8(d)	3330.6,3433.9,3501.8,3514.1,3519.9,3565.6,3588.1,3608.8,3642.4,3646.8,3691.5,3713.8, 3723.7,3732.5,3862.1,3880.3
8(e)	3003.8,3373.4,3417.6,3494.8,3523.5,3553.3,3570.7,3609.0,3631.0,3642.2,3676.2,3685.4, 3698.9,3717.0,3869.3,3879.5
8(f)	3430.8,3434.2,3493.6,3504.5,3520.6,3533.6,3542.3,3573.4,3628.6,3641.8,3713.5,3745.3, 3749.4,3750.2,3764.1,3775.4
8(g)	3049.3,3312.8,3455.2,3462.8,3498.6,3558.4,3562.9,3620.4,3636.3,3644.2,3669.4,3673.5, 3699.8,3736.6,3866.5,3883.3
8(h)	3194.3,3330.9,3432.2,3484.3,3520.0,3529.3,3558.4,3628.5,3674.2,3675.3,3679.6,3698.1, 3715.9,3844.6,3860.6,3882.9
8(i)	3487.6,3499.8,3514.3,3529.0,3549.1,3558.0,3574.0,3580.6,3603.1,3621.9,3658.8,3662.3, 3673.8,3698.1,3865.3,3865.7
8(j)	3373.8,3376.5,3485.2,3496.3,3521.1,3522.5,3556.1,3596.6,3627.6,3638.5,3647.2,3696.5, 3767.8,3773.3,3863.7,3877.1
8(k)	3263.4,3376.1,3464.6,3507.0,3567.7,3582.8,3653.6,3659.7,3681.0,3691.0,3709.4,3716.4, 3729.6,3798.5,3809.2,3879.6
8(l)	3266.9,3478.8,3499.0,3518.4,3557.3,3581.4,3602.8,3647.8,3658.0,3682.9,3709.5,3729.8, 3734.6,3737.5,3792.1,3879.4
8(m)	3150.8,3239.9,3429.3,3503.1,3560.4,3574.3,3606.4,3615.9,3647.7,3663.9,3697.9,3718.8, 3753.0,3839.4,3877.8,3880.5
8(n)	3073.4,3320.0,3427.7,3464.8,3509.1,3536.0,3547.4,3622.2,3645.4,3667.8,3737.2,3777.0,

	3782.3,3795.9,3803.8,3883.3
8(o)	3341.4,3404.8,3496.9,3555.1,3577.0,3588.8,3615.5,3623.6,3626.8,3676.4,3687.9,3703.8, 3730.4,3740.5,3762.2,3868.2
8(p)	3457.7,3458.4,3523.2,3526.0,3541.9,3545.4,3576.3,3580.8,3748.1,3749.4,3750.4,3755.1, 3762.7,3769.9,3783.5,3788.4
8(q)	3208.3,3270.1,3430.4,3532.8,3558.6,3576.7,3588.5,3627.1,3634.5,3642.0,3705.8,3709.6, 3722.1,3869.3,3878.1,3878.3
8(r)	3335.6,3456.7,3507.5,3527.9,3556.8,3564.1,3588.0,3609.3,3615.6,3642.2,3663.4,3675.5, 3683.8,3790.6,3873.2,3877.2
8(s)	3410.9,3472.3,3490.9,3528.6,3533.8,3566.9,3582.7,3600.6,3610.7,3626.6,3638.3,3681.0, 3704.4,3766.1,3874.7,3880.6
8(t)	3115.7,3217.4,3369.5,3522.2,3565.7,3599.7,3611.2,3632.7,3644.8,3662.7,3700.6,3711.2, 3797.3,3871.0,3879.5,3883.3
8(u)	3207.1,3383.0,3396.9,3436.6,3494.1,3543.6,3593.9,3607.2,3657.4,3670.4,3705.7,3722.8, 3753.1,3870.3,3876.4,3882.6
8(v)	3354.3,3383.5,3449.5,3521.4,3524.4,3556.1,3557.2,3578.6,3639.9,3642.4,3783.1,3784.7, 3789.5,3797.1,3868.0,3868.3
8(w)	3145.9,3242.6,3408.8,3435.7,3452.2,3510.4,3537.2,3598.7,3627.6,3642.2,3673.3,3697.7, 3738.3,3815.8,3869.7,3889.1
8(x)	3421.4,3423.2,3488.9,3489.5,3514.5,3515.1,3529.8,3548.0,3740.5,3743.2,3744.6,3757.3, 3770.5,3776.4,3776.6,3785.2
8(y)	3385.4,3393.6,3437.6,3499.9,3536.1,3567.3,3574.2,3596.2,3662.9,3723.3,3749.3,3762.1, 3774.1,3862.4,3868.5,3876.9
8(z)	3359.0,3465.5,3496.6,3560.0,3601.3,3657.0,3667.1,3677.7,3702.7,3713.5,3720.1,3732.1, 3746.0,3868.7,3872.8,3876.1
8(aa)	3183.6,3364.4,3425.8,3460.0,3539.2,3552.8,3563.2,3613.8,3654.0,3675.2,3693.7,3714.5, 3727.9,3741.5,3872.7,3881.7
8(bb)	3151.7,3272.3,3391.6,3430.0,3545.5,3577.2,3604.7,3645.5,3665.7,3694.6,3752.8,3813.8, 3835.2,3872.9,3881.9,3886.4