

SUPPORTING INFORMATION

**pH-Controlled Twisted Intramolecular Charge Transfer
(TICT) Excited State via Changing the Intramolecular
Charge Transfer Direction**

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Table S1. Cartesian coordinates of the optimized geometric conformations for various forms of the isolated MIR at different pH values.

KETO (Isomer I)

S₀ state

25

C	-8.6203983	3.9649378	-0.6657543
C	-7.4216054	3.2617023	-0.6377328
C	-7.3211472	2.1074195	0.1449878
C	-8.4570849	1.7361663	0.8697236
C	-9.6118021	2.5043418	0.7683421
N	-9.7082630	3.6026847	0.0172438
C	-6.0450261	1.3536968	0.2260608
C	-4.8480894	2.0547343	0.5330784
C	-3.6258462	1.4426776	0.6452659
C	-3.4957299	0.0040243	0.4424231
N	-4.7273566	-0.6004360	0.1193024
C	-5.9477820	-0.0055155	0.0064928
H	-8.7128917	4.8602427	-1.2722945
H	-6.5823671	3.6034011	-1.2310651
H	-8.4411739	0.8754189	1.5261438
H	-10.5002125	2.2274323	1.3272728
H	-4.9082862	3.1232064	0.7026338
C	-2.4575211	2.1892233	0.9673448
O	-2.4849482	-0.6674505	0.5174183
H	-4.6483826	-1.5955184	-0.0521675
C	-7.0733913	-0.9186554	-0.3800506
H	-7.9268612	-0.3593561	-0.7541888
H	-7.4060532	-1.5119920	0.4768738
H	-6.7473812	-1.6140017	-1.1574561
N	-1.5272083	2.8204194	1.2277865

KETO (Isomer I)

S₁ state

25

C	-2.2666858	2.6051974	-0.7950115
C	-1.0524257	1.9305143	-0.7595700
C	-0.9459404	0.7536882	-0.0079364
C	-2.0940379	0.3277859	0.6723945
C	-3.2558955	1.0827669	0.5803573
N	-3.3586727	2.2022862	-0.1413996
C	0.3351341	0.0266188	0.0854214
C	1.4941292	0.7362125	0.3687973
C	2.7673605	0.0638071	0.4703272
C	2.7949144	-1.3490074	0.4236176
N	1.5829398	-2.0050174	0.2353569
C	0.3957309	-1.3905678	-0.0980790
H	-2.3684542	3.5121986	-1.3822025
H	-0.2067762	2.3009706	-1.3250043
H	-2.0738026	-0.5601558	1.2920442
H	-4.1491209	0.7748925	1.1146355
H	1.4501295	1.8003556	0.5478042
C	3.9529785	0.7801685	0.7143583
O	3.8056568	-2.0851269	0.5344859
H	1.6689486	-3.0112015	0.1589635
C	-0.6577058	-2.2689339	-0.6785697
H	-1.5401608	-1.7011853	-0.9606732
H	-0.9721960	-3.0541715	0.0231255
H	-0.2869847	-2.7799741	-1.5775565
N	4.9032673	1.4170558	0.9060204

KETO (Isomer II)

S₀ state

25

C	-8.9382145	3.8038408	0.8031058
C	-7.7392363	3.1130062	0.9333079
C	-7.4398976	2.0816751	0.0373505
C	-8.3854316	1.8170013	-0.9573037
C	-9.5587601	2.5620606	-0.9985755
N	-9.8461391	3.5415061	-0.1396157
C	-6.1524862	1.3494814	0.1293823
C	-4.9431433	2.0900798	0.2114262
C	-3.7052897	1.5048067	0.2913921
C	-3.5722165	0.0526630	0.3065053
N	-4.8222429	-0.5957669	0.2359588
C	-6.0573201	-0.0276123	0.1518785
H	-9.1837500	4.6042875	1.4937095
H	-7.0552691	3.3681826	1.7336047
H	-8.2051162	1.0599755	-1.7100422
H	-10.2996871	2.3680926	-1.7677440
H	-5.0021312	3.1716606	0.1912969
C	-2.5246041	2.2975725	0.3524873
O	-2.5481752	-0.5991491	0.3745032
H	-4.7473783	-1.6053174	0.2663771
C	-7.2064822	-0.9911436	0.1087330
H	-8.1339122	-0.5158722	0.4180599
H	-7.0162161	-1.8418911	0.7664782
H	-7.3484307	-1.3817930	-0.9031609
N	-1.5883155	2.9707412	0.3988287

KETO (Isomer II)

S₁ state

25

C	-8.9812661	3.8120687	0.7813222
C	-7.7635372	3.1557647	0.9133477
C	-7.4498354	2.1129306	0.0326158
C	-8.4017236	1.7996035	-0.9463517
C	-9.5829124	2.5275278	-1.0010957
N	-9.8863697	3.5152143	-0.1540120
C	-6.1563713	1.4079767	0.1176328
C	-4.9883447	2.1495199	0.2240186
C	-3.7025065	1.4985425	0.2966832
C	-3.6373175	0.0982189	0.1094221
N	-4.8390571	-0.5750699	-0.0871985
C	-6.0898887	-0.0209202	0.0742403
H	-9.2450785	4.6133138	1.4642130
H	-7.0769738	3.4347819	1.7023306
H	-8.2099482	1.0241181	-1.6773240
H	-10.3220511	2.3096476	-1.7654577
H	-5.0271109	3.2288552	0.2175281
C	-2.5183271	2.2441302	0.4400882
O	-2.6026203	-0.6113459	0.1005736
H	-4.7387414	-1.5800831	-0.1622881
C	-7.2188127	-0.9783070	0.2409161
H	-8.1483495	-0.4621541	0.4658158
H	-7.0168019	-1.6771782	1.0636084
H	-7.3820864	-1.5884914	-0.6588204
N	-1.5764358	2.9085602	0.5691709

ENOL (Isomer I)

S₀ state

25

C	-2.4780934	2.3780897	-0.9895925
C	-1.2478656	1.7312731	-0.9503830
C	-1.0722207	0.6445185	-0.0891018
C	-2.1679594	0.2753893	0.6953070
C	-3.3569780	0.9863699	0.5808092
N	-3.5256571	2.0224616	-0.2434453
C	0.2389124	-0.0479734	0.0059046
C	1.3892081	0.7055311	0.2433419
C	2.6381256	0.0999596	0.3499443
C	2.6747097	-1.2997247	0.2075692
N	1.5989958	-2.0222897	-0.0395522
C	0.3962090	-1.4397374	-0.1459967
H	-2.6297303	3.2208088	-1.6568634
H	-0.4424299	2.0629411	-1.5944228
H	-2.0965843	-0.5416494	1.4018439
H	-4.2149502	0.7131440	1.1872043
H	1.3155100	1.7789751	0.3630532
C	3.8162015	0.8593356	0.6013145
O	3.8524889	-1.9344940	0.3177689
C	-0.7387773	-2.3752406	-0.4575104
H	-1.5527824	-1.8775823	-0.9816422
H	-1.1463848	-2.8040968	0.4629357
H	-0.3650726	-3.2018182	-1.0605648
N	4.7576386	1.4944127	0.8059296
H	3.6811428	-2.8793528	0.1852591

ENOL (Isomer I)

S₁ state

25

C	-2.4372343	2.5089271	-0.7408084
C	-1.2053850	1.8769815	-0.7413483
C	-1.0630362	0.6150571	-0.1072305
C	-2.2203575	0.1138740	0.5371225
C	-3.3952346	0.8403364	0.4942818
N	-3.5233779	2.0197434	-0.1334811
C	0.2177134	-0.0566913	-0.0829078
C	1.3979893	0.7599407	-0.0898415
C	2.6591365	0.1266376	0.1167597
C	2.6405821	-1.2929701	0.2262964
N	1.5698045	-2.0660522	0.1086818
C	0.3511553	-1.4793518	-0.0547085
H	-2.5611421	3.4623098	-1.2435532
H	-0.3688451	2.3250332	-1.2587306
H	-2.1816372	-0.8052200	1.1028787
H	-4.2831221	0.4729813	0.9973963
H	1.3267211	1.8322796	0.0025974
C	3.8433257	0.8561262	0.3009849
O	3.7961083	-1.9120411	0.4684785
C	-0.7420741	-2.4577283	-0.3563721
H	-1.6335720	-2.0009885	-0.7769771
H	-1.0226491	-3.0223049	0.5421668
H	-0.3604485	-3.1963032	-1.0672508
N	4.8029610	1.4985500	0.4367283
H	3.5951225	-2.8622944	0.5247319

ENOL (Isomer II)

S₀ state

25

C	-9.0109338	3.7390533	0.7864970
C	-7.8022601	3.0709062	0.9470190
C	-7.4314345	2.0932680	0.0192488
C	-8.3182314	1.8505473	-1.0325978
C	-9.5052714	2.5707604	-1.1017256
N	-9.8609562	3.5018501	-0.2142946
C	-6.1298185	1.3865057	0.1377081
C	-4.9605381	2.1377882	0.2625376
C	-3.7167709	1.5226150	0.3702057
C	-3.7048053	0.1156473	0.3412350
N	-4.8036511	-0.6078249	0.2471240
C	-6.0029799	-0.0167705	0.1492796
H	-9.3126050	4.4994837	1.4999420
H	-7.1659050	3.3013915	1.7929160
H	-8.0844723	1.1257260	-1.8020689
H	-10.2017795	2.3953952	-1.9156174
H	-5.0122742	3.2191271	0.2635238
C	-2.5178195	2.2787602	0.5032396
O	-2.5287162	-0.5261791	0.4226421
C	-7.1713739	-0.9604204	0.0778441
H	-8.0823553	-0.5253100	0.4852961
H	-6.9264527	-1.8715327	0.6222149
H	-7.3725468	-1.2453515	-0.9592192
N	-1.5571829	2.9077494	0.6169294
H	-2.7191752	-1.4762810	0.3961540

ENOL (Isomer II)

S₁ state

25

C	-8.8969151	3.8883108	0.6729322
C	-7.6887360	3.2277224	0.8182825
C	-7.4150445	2.0814625	0.0266605
C	-8.4146342	1.7265588	-0.9113992
C	-9.5743056	2.4736529	-0.9905301
N	-9.8324190	3.5394192	-0.2165168
C	-6.1533807	1.3848312	0.1484654
C	-5.0033476	2.1539380	0.5315709
C	-3.7231029	1.5276001	0.4762316
C	-3.7125608	0.1452478	0.1357849
N	-4.7810931	-0.6045529	-0.0976789
C	-6.0096250	-0.0162065	-0.0936361
H	-9.1261365	4.7490365	1.2924047
H	-6.9780872	3.5600743	1.5618624
H	-8.2595967	0.9091153	-1.5993927
H	-10.3371246	2.2214234	-1.7190978
H	-5.0605479	3.2280934	0.6104160
C	-2.5294579	2.2435001	0.6533334
O	-2.5300952	-0.4629064	0.0406372
C	-7.1357780	-0.9979018	-0.2037558
H	-8.0942858	-0.6019935	0.1207517
H	-6.8937952	-1.8722495	0.4067943
H	-7.2360710	-1.3675925	-1.2325651
N	-1.5645778	2.8711977	0.8176495
H	-2.7129362	-1.3852218	-0.2094600

ANION (Isomer I)

S_0 state

24

C	-8.6256295	4.1042291	-0.2400368
C	-7.4283205	3.4090285	-0.2886209
C	-7.3380641	2.1001828	0.2281789
C	-8.5362995	1.6017235	0.7743230
C	-9.6867482	2.3763156	0.7664140
N	-9.7634309	3.6172157	0.2717809
C	-6.0713683	1.3631504	0.2213133
C	-4.8726713	2.0606791	0.4288546
C	-3.6494603	1.4198426	0.4602486
C	-3.5757980	-0.0357204	0.2829410
N	-4.7799919	-0.6777587	0.0046999
C	-5.9312622	-0.0422552	-0.0089296
H	-8.6810915	5.1107207	-0.6471658
H	-6.5655588	3.8721225	-0.7509206
H	-8.5661065	0.6231892	1.2323647
H	-10.6035707	1.9794998	1.1954800
H	-4.9024112	3.1302122	0.6069787
C	-2.4678117	2.1669403	0.7086945
O	-2.5197485	-0.6679461	0.3626148
C	-7.1137667	-0.9207327	-0.3693904
H	-7.8702746	-0.3928453	-0.9524054
H	-7.6012046	-1.3162121	0.5277267
H	-6.7379759	-1.7716177	-0.9357213
N	-1.5267317	2.8117960	0.9109020

ANION (Isomer II)

S₀ state

24

C	-8.7843913	3.9179963	1.0942419
C	-7.5997487	3.2006143	1.1168748
C	-7.3935143	2.1280790	0.2245265
C	-8.4696133	1.8771636	-0.6484767
C	-9.6191931	2.6504285	-0.5852255
N	-9.8056049	3.6666205	0.2648908
C	-6.1309942	1.3843523	0.2048691
C	-4.9313877	2.0658773	0.4578369
C	-3.7063955	1.4288812	0.4245830
C	-3.6289264	-0.0014158	0.1028267
N	-4.8470715	-0.6550643	-0.0641052
C	-5.9986705	-0.0207710	-0.0325470
H	-8.9308736	4.7383931	1.7922936
H	-6.8403759	3.4555310	1.8454774
H	-8.4007246	1.1002954	-1.3965776
H	-10.4397768	2.4482951	-1.2693533
H	-4.9552634	3.1327783	0.6510061
C	-2.5171400	2.1684180	0.6588288
O	-2.5597855	-0.6064809	-0.0072061
C	-7.2031861	-0.9281643	-0.1963567
H	-7.5044778	-0.9982999	-1.2467349
H	-8.0690745	-0.5911709	0.3757926
H	-6.9145414	-1.9278763	0.1256195
N	-1.5686433	2.8028393	0.8591310

ANION
TICT state

24

C	-9.1087683	3.4159254	-0.9081158
C	-7.8915929	2.7834739	-0.9711239
C	-7.3476157	2.1616195	0.1956773
C	-8.1634835	2.2439300	1.3666204
C	-9.3677661	2.9021638	1.3192578
N	-9.9020930	3.5184109	0.2111627
C	-6.0444535	1.4489298	0.1803272
C	-4.8569720	2.1019152	0.4694765
C	-3.6420089	1.4171464	0.4467407
C	-3.6229167	-0.0065486	0.1086997
N	-4.8213875	-0.6386598	-0.1745287
C	-5.9451307	0.0360883	-0.1396193
H	-9.5041377	3.8914025	-1.8031635
H	-7.3500023	2.7718460	-1.9121508
H	-7.8408773	1.7986885	2.3029366
H	-9.9717538	2.9643081	2.2219376
H	-4.8832340	3.1554398	0.7151207
C	-2.4240444	2.0752198	0.7472842
O	-2.5575736	-0.6400676	0.0752641
C	-7.2048147	-0.7209908	-0.4547520
H	-7.7225887	-0.2690452	-1.3028939
H	-7.9023461	-0.6678722	0.3834333
H	-6.9591840	-1.7586074	-0.6733959
N	-1.4474290	2.6408886	1.0014561

CATION (Isomer I)

S₀ state

26

C	-2.3961135	2.5240681	-0.8133051
C	-1.2012560	1.8533022	-0.7721111
C	-1.0861846	0.6207442	-0.0910486
C	-2.2510636	0.1299848	0.5369748
C	-3.4274217	0.8329940	0.4768362
N	-3.4796122	2.0053886	-0.1935406
C	0.2020021	-0.0685999	-0.0133786
C	1.3612855	0.7050491	0.1694648
C	2.6046260	0.1152534	0.2936766
C	2.6464887	-1.2973466	0.2112667
N	1.5676794	-2.0331773	-0.0067197
C	0.3627077	-1.4746216	-0.1162132
H	-2.5343433	3.4619231	-1.3328281
H	-0.3565825	2.2764757	-1.2969371
H	-2.2301342	-0.7855498	1.1080491
H	-4.3384168	0.5076935	0.9595490
H	1.2933972	1.7813662	0.2611616
C	3.7755546	0.8940012	0.5182636
O	3.8156915	-1.9043622	0.3506138
C	-0.7504013	-2.4420480	-0.4117498
H	-1.5727950	-1.9934219	-0.9672364
H	-1.1476081	-2.8662983	0.5158553
H	-0.3467845	-3.2724243	-0.9888264
N	4.7022648	1.5549703	0.7011863
H	3.6859366	-2.8629996	0.2629721
H	-4.3565220	2.5129526	-0.2296346

CATION (Isomer II)

S₀ state

26

C	-8.9127234	3.8731178	0.7311152
C	-7.7322729	3.1893162	0.8711822
C	-7.4361599	2.0814028	0.0461820
C	-8.4048123	1.7288031	-0.9179230
C	-9.5717067	2.4412048	-1.0305262
N	-9.8043549	3.4895267	-0.2095958
C	-6.1585643	1.3777730	0.1698718
C	-4.9937458	2.1361454	0.3811796
C	-3.7518689	1.5338273	0.4528631
C	-3.7217427	0.1249638	0.3175271
N	-4.8168889	-0.6033949	0.1713626
C	-6.0178248	-0.0313897	0.0916475
H	-9.1888770	4.7163071	1.3487271
H	-7.0469816	3.4995807	1.6474357
H	-8.2316083	0.9167655	-1.6076153
H	-10.3335694	2.2204101	-1.7649870
H	-5.0456706	3.2153572	0.4463465
C	-2.5587950	2.2921835	0.6230430
O	-2.5463622	-0.4859393	0.3465552
C	-7.1641916	-0.9987756	-0.0160583
H	-8.1060985	-0.5918848	0.3478273
H	-6.9220452	-1.8919095	0.5580589
H	-7.2990857	-1.3192148	-1.0537901
N	-1.6049446	2.9257025	0.7572084
H	-2.6852533	-1.4422468	0.2504039
H	-10.6713549	4.0063889	-0.3055509

CATION
TICT state

26

C	-2.8072587	1.7727701	-1.4258753
C	-1.5986178	1.1523106	-1.3381626
C	-1.1117377	0.6794676	-0.0929224
C	-1.9164650	0.8966990	1.0539300
C	-3.1233532	1.5192475	0.9530038
N	-3.5805567	1.9478100	-0.2862008
C	0.2265150	0.0194171	0.0103192
C	1.3652737	0.7625172	0.2273511
C	2.6173757	0.1326976	0.3172915
C	2.6337900	-1.3059611	0.1745592
N	1.5483427	-2.0355126	-0.0364044
C	0.3720325	-1.4281765	-0.1205726
H	-3.2157406	2.1495133	-2.3498497
H	-1.0224842	1.0363829	-2.2462473
H	-1.5927950	0.5781184	2.0356184
H	-3.7669770	1.7064181	1.7975408
H	1.3050545	1.8377436	0.3290291
C	3.8087763	0.8419575	0.5362174
O	3.7933440	-1.9027959	0.2620864
C	-0.8157842	-2.2884254	-0.3473214
H	-1.3922016	-1.9359942	-1.2055542
H	-1.4935090	-2.2208823	0.5098395
H	-0.5131692	-3.3216144	-0.4916021
N	4.7866053	1.4369854	0.7189474
H	3.6762282	-2.8663249	0.1520033
H	-4.4683955	2.4159793	-0.3548016

Table S2. Cartesian coordinates of the optimized geometric conformations of the hydrogen-bonded complexes with water molecules in the first solvation shell for various forms of MIR

KETO-3H₂O (Isomer I)

S₀ state

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C	-8.6689232	3.8853944	-0.7056716
C	-7.4545715	3.2139358	-0.6513688
C	-7.3358570	2.0725595	0.1474290
C	-8.4661740	1.6857998	0.8732022
C	-9.6386674	2.4208629	0.7539557
N	-9.7508059	3.4994490	-0.0246670
C	-6.0495054	1.3367450	0.2330561
C	-4.8666113	2.0421826	0.5580577
C	-3.6378591	1.4321307	0.6536300
C	-3.5049776	0.0072321	0.4103626
N	-4.7173789	-0.6090249	0.0784006
C	-5.9360359	-0.0210783	-0.0170052
H	-8.7838222	4.7672047	-1.3268379
H	-6.6193521	3.5684539	-1.2423544
H	-8.4334332	0.8346989	1.5411172
H	-10.5246468	2.1385860	1.3129867
H	-4.9350920	3.1059044	0.7535196
C	-2.4699040	2.1725737	0.9869062
O	-2.4669424	-0.6458845	0.4646278
H	-4.6206913	-1.6097411	-0.1320573
C	-7.0573657	-0.9342451	-0.4186779
H	-7.8898206	-0.3793173	-0.8436912
H	-7.4279992	-1.4926808	0.4454768
H	-6.7086487	-1.6638616	-1.1519855
N	-1.5353744	2.7959243	1.2466606
O	-12.2753796	4.9567562	-0.3648113
H	-11.4334450	4.4874230	-0.2118956
H	-12.6929968	4.4882294	-1.0940989
O	0.8730734	4.6636121	1.5087737
H	0.0933239	4.0904432	1.5444104
H	1.4239584	4.2742151	0.8225901
O	-3.5196958	-3.1210346	-0.1917057
H	-3.1584081	-3.7799870	-0.7922780
H	-2.7948731	-2.5088500	0.0411630

KETO-3H₂O (Isomer I)

S₁ state

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C	-8.6978761	3.9059960	-0.6443760
C	-7.4704523	3.2586102	-0.6266096
C	-7.3360743	2.0605894	0.0891527
C	-8.4716204	1.5902544	0.7637473
C	-9.6514359	2.3165769	0.6950436
N	-9.7765449	3.4503425	-0.0016766
C	-6.0385600	1.3639445	0.1508348
C	-4.8957186	2.1110507	0.4267201
C	-3.6151762	1.4619325	0.5521740
C	-3.5468863	0.0510849	0.4236588
N	-4.7155983	-0.6330384	0.1486476
C	-5.9423478	-0.0476727	-0.0547866
H	-8.8261472	4.8293280	-1.1989711
H	-6.6344471	3.6664874	-1.1797037
H	-8.4297320	0.6899543	1.3625864
H	-10.5368359	1.9800498	1.2236017
H	-4.9698994	3.1703569	0.6220134
C	-2.4553146	2.1878882	0.8640859
O	-2.4954326	-0.6341751	0.5388732
H	-4.5945843	-1.6450464	0.0208251
C	-7.0202458	-0.9604231	-0.5310765
H	-7.9010337	-0.4112674	-0.8518945
H	-7.3280066	-1.6726134	0.2468914
H	-6.6684237	-1.5593366	-1.3796466
N	-1.5283733	2.8386188	1.1136436
O	-12.2325066	5.0655255	-0.0506493
H	-11.4244352	4.5202274	-0.0128105
H	-12.7108438	4.7523504	-0.8243525
O	0.7827600	4.7385872	1.4855822
H	-0.0044176	4.1803513	1.3886802
H	1.5168744	4.1165588	1.4945857
O	-3.5961885	-3.2300707	0.0987805
H	-3.3193981	-3.9409147	-0.4882473
H	-2.8055529	-2.7048013	0.3011409

KETO-3H₂O (Isomer II)

S₀ state

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C	-9.4029522	2.7329105	-0.9369544
C	-8.2144127	2.0141221	-0.9501235
C	-7.3684032	2.0649747	0.1613101
C	-7.7746404	2.8660699	1.2331443
C	-8.9791370	3.5528113	1.1527855
N	-9.7894672	3.4899471	0.0934322
C	-6.0734316	1.3408035	0.2041732
C	-4.8900910	2.0555226	0.5060655
C	-3.6522202	1.4593075	0.5597375
C	-3.5115340	0.0365849	0.3115415
N	-4.7294323	-0.5957488	0.0359791
C	-5.9569147	-0.0206467	-0.0212599
H	-10.0729133	2.7146434	-1.7900983
H	-7.9445825	1.4427428	-1.8289998
H	-7.1702260	2.9438739	2.1284530
H	-9.3114013	4.1765380	1.9756977
H	-4.9605389	3.1213026	0.6880763
C	-2.4842488	2.2149494	0.8546563
O	-2.4655700	-0.6059709	0.3351984
H	-4.6358335	-1.6065992	-0.1207226
C	-7.0907027	-0.9611139	-0.3062202
H	-8.0422958	-0.5448215	0.0141172
H	-6.9309697	-1.9107511	0.2076775
H	-7.1575724	-1.1737682	-1.3771437
N	-1.5534021	2.8511418	1.0951695
O	-12.2474015	4.7279178	-0.8879312
H	-11.4516369	4.4153403	-0.4178974
H	-12.9901922	4.3728631	-0.3900682
O	0.7800231	4.7784563	1.5326449
H	0.0018092	4.2107907	1.4324191
H	1.5235563	4.2039708	1.3256433
O	-3.5314199	-3.1287267	-0.0916769
H	-3.1963292	-3.8049437	-0.6884181
H	-2.8050115	-2.4940792	0.0638392

KETO-3H₂O (Isomer II)

S₁ state

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C	-9.4129464	2.6920173	-0.9292062
C	-8.2259844	1.9744302	-0.9205604
C	-7.3717001	2.0745459	0.1858500
C	-7.7814375	2.9085043	1.2352853
C	-8.9942833	3.5760064	1.1380559
N	-9.8041688	3.4757707	0.0812630
C	-6.0746767	1.3766884	0.2465372
C	-4.9441959	2.1099600	0.6030452
C	-3.6444683	1.4867176	0.6053706
C	-3.5449300	0.1119419	0.2722659
N	-4.7059786	-0.5661208	-0.0444152
C	-5.9648964	-0.0148097	-0.0566844
H	-10.0842538	2.6456597	-1.7797358
H	-7.9549082	1.3742726	-1.7792490
H	-7.1722944	3.0156049	2.1234236
H	-9.3347028	4.2165906	1.9442961
H	-5.0199867	3.1689940	0.7976313
C	-2.4807946	2.2228781	0.8734599
O	-2.4712803	-0.5486822	0.2510018
H	-4.5765563	-1.5697611	-0.2201096
C	-7.0812120	-0.9679324	-0.3185261
H	-8.0480758	-0.5273872	-0.0908144
H	-6.9670114	-1.8696876	0.2941065
H	-7.0999643	-1.3007568	-1.3657296
N	-1.5542032	2.8822110	1.1011343
O	-12.2733254	4.6667307	-0.9339543
H	-11.4768417	4.3744140	-0.4528873
H	-13.0144652	4.3854806	-0.3887872
O	0.7583118	4.7723439	1.5453628
H	-0.0316304	4.2204173	1.4357657
H	1.4901449	4.1849142	1.3328917
O	-3.5671930	-3.1422203	-0.1619696
H	-3.3270148	-3.8909751	-0.7165219
H	-2.7647945	-2.6115546	-0.0326289

ENOL-3H₂O (Isomer I)

S₀ state

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C	-2.5261095	2.2994885	-1.0299988
C	-1.2874279	1.6707272	-1.0099744
C	-1.0820183	0.5872666	-0.1511879
C	-2.1547954	0.2045087	0.6588990
C	-3.3564933	0.8942934	0.5682998
N	-3.5509780	1.9219780	-0.2618598
C	0.2372089	-0.0927696	-0.0823308
C	1.3820640	0.6656596	0.1694123
C	2.6310923	0.0651465	0.2648758
C	2.6980076	-1.3371005	0.1002944
N	1.6135429	-2.0576770	-0.1740730
C	0.4072633	-1.4763248	-0.2695321
H	-2.7093064	3.1399751	-1.6909465
H	-0.4986991	2.0139494	-1.6679708
H	-2.0542446	-0.6074699	1.3675471
H	-4.1987457	0.6167794	1.1931382
H	1.3003923	1.7361321	0.3106961
C	3.8039426	0.8263272	0.5279759
O	3.8761439	-1.9329844	0.2160278
C	-0.7224962	-2.4086152	-0.6116691
H	-0.3660184	-3.1706500	-1.3048920
H	-1.0778943	-2.9255166	0.2847379
H	-1.5683526	-1.8892747	-1.0570069
N	4.7432871	1.4614284	0.7353590
H	3.7788405	-2.9131814	0.0937685
O	-5.9237134	3.6060780	-0.6118745
H	-6.4674523	3.1209902	-1.2401284
H	-5.1663358	3.0188392	-0.4262405
O	3.0864556	-4.4760825	-0.1313846
H	2.2412702	-4.0190241	-0.3020329
H	3.2592849	-5.0606213	-0.8770442
O	7.1389255	3.3582315	0.8828328
H	7.8371943	2.7665795	0.5857638
H	6.3458770	2.8031045	0.9076861

ENOL-3H₂O (Isomer I)

S₁ state

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C	-2.5064479	2.3827019	-0.8041423
C	-1.2554022	1.7892173	-0.7966028
C	-1.0848527	0.5213936	-0.1915586
C	-2.2281058	-0.0323008	0.4271277
C	-3.4278334	0.6538358	0.3853837
N	-3.5827672	1.8352774	-0.2284753
C	0.2179532	-0.1196609	-0.1731111
C	1.3703773	0.7195663	-0.0938556
C	2.6462600	0.1058433	0.0684397
C	2.6820702	-1.3227171	0.0715130
N	1.6150781	-2.1088388	-0.1107327
C	0.3825570	-1.5388687	-0.2380778
H	-2.6605182	3.3423181	-1.2851156
H	-0.4259970	2.2776273	-1.2888596
H	-2.1656798	-0.9629829	0.9715264
H	-4.3093002	0.2488223	0.8698518
H	1.2699008	1.7832504	0.0534372
C	3.8104151	0.8509005	0.2982503
O	3.8521882	-1.8974870	0.2611926
C	-0.6941544	-2.5182568	-0.5927048
H	-0.3120476	-3.2021692	-1.3567625
H	-0.9622508	-3.1419626	0.2699683
H	-1.5967971	-2.0526680	-0.9776262
N	4.7520807	1.5090017	0.4728389
H	3.7539341	-2.8989388	0.2451214
O	-5.8149728	3.7256608	-0.5806631
H	-6.3770985	3.3688925	-1.2752590
H	-5.1682330	3.0230106	-0.3878506
O	3.1257776	-4.4225949	0.1473008
H	2.2682173	-3.9961466	-0.0604668
H	3.3334539	-5.0365010	-0.5655402
O	7.0859049	3.3659777	0.8738194
H	7.7935462	2.7278722	1.0076544
H	6.2934710	2.8223111	0.7407820

ENOL-3H₂O (Isomer II)

S₀ state

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C	-3.1089682	1.1635592	-1.3038175
C	-1.8965253	0.4871500	-1.2699675
C	-1.0840603	0.5942529	-0.1385494
C	-1.5472660	1.3985327	0.9061811
C	-2.7748826	2.0370379	0.7812448
N	-3.5513494	1.9249442	-0.2987883
C	0.2356758	-0.0833752	-0.0508004
C	1.3814145	0.6797998	0.1781848
C	2.6340195	0.0831766	0.2558119
C	2.7023291	-1.3196775	0.0980572
N	1.6086271	-2.0514822	-0.1002470
C	0.3985464	-1.4746869	-0.1722025
H	-3.7548565	1.1044543	-2.1734601
H	-1.5831577	-0.0982097	-2.1250157
H	-0.9671352	1.5163638	1.8129833
H	-3.1535810	2.6622301	1.5827901
H	1.3023618	1.7546531	0.2833070
C	3.8095019	0.8544103	0.4747057
O	3.8890152	-1.9073171	0.1590151
C	-0.7513456	-2.4246410	-0.3662344
H	-0.8639769	-2.6803320	-1.4241411
H	-0.5525365	-3.3502740	0.1740235
H	-1.6952314	-2.0064227	-0.0227893
N	4.7476228	1.5009030	0.6500244
H	3.7922397	-2.8891774	0.0499717
O	-6.0278225	3.0313348	-1.3769232
H	-6.7659553	2.6385975	-0.9008189
H	-5.2321750	2.7650266	-0.8784635
O	3.0931149	-4.4558795	-0.1359607
H	2.2393365	-3.9972438	-0.2535970
H	3.2219245	-5.0337147	-0.8955968
O	7.1185229	3.4087460	0.9425213
H	7.8560845	2.7910169	0.9415914
H	6.3324368	2.8485320	0.8645796

ENOL-3H₂O (Isomer II)

S₁ state

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C	-3.2272749	0.9257155	-1.0827197
C	-2.0465210	0.2093293	-1.0131725
C	-1.0737567	0.5541397	-0.0477200
C	-1.3846043	1.6571448	0.7840004
C	-2.6054410	2.2950211	0.6483159
N	-3.5191721	1.9484901	-0.2644940
C	0.2067672	-0.1191503	0.0703177
C	1.3364198	0.6685729	0.4493176
C	2.6246799	0.0613639	0.4269725
C	2.6817161	-1.3258424	0.0882522
N	1.6141960	-2.0870610	-0.1754370
C	0.3743929	-1.5172078	-0.1774742
H	-3.9805405	0.6897182	-1.8262505
H	-1.8598815	-0.5767035	-1.7298193
H	-0.6920373	1.9775443	1.5497439
H	-2.8639054	3.1263205	1.2949276
H	1.2564088	1.7399365	0.5445404
C	3.7989745	0.7944523	0.6423802
O	3.8728220	-1.8870910	0.0432824
C	-0.7389125	-2.5108432	-0.3081638
H	-0.8067100	-2.8985492	-1.3334341
H	-0.5202868	-3.3718553	0.3308672
H	-1.7102337	-2.1157567	-0.0243099
N	4.7430403	1.4440289	0.8355151
H	3.7892833	-2.8598886	-0.1984246
O	-6.0251114	2.5569138	-1.6015098
H	-6.8017682	2.7767349	-1.0781669
H	-5.2751212	2.5746064	-0.9807567
O	3.1659902	-4.3590232	-0.5170805
H	2.2879268	-3.9234557	-0.5377118
H	3.2858992	-4.8254030	-1.3514291
O	7.0438313	3.3892672	0.9047726
H	7.7772629	2.7891855	1.0717865
H	6.2625141	2.8142579	0.8861493

ANION-3H₂O (Isomer I)

S₀ state

33

C	-8.6823531	4.0816159	-0.2717853
C	-7.4803015	3.3969492	-0.3180234
C	-7.3797492	2.0946857	0.2087642
C	-8.5653187	1.5817928	0.7660462
C	-9.7242531	2.3408321	0.7612606
N	-9.8063913	3.5763203	0.2525609
C	-6.1038369	1.3695880	0.2025792
C	-4.9182334	2.0729457	0.4504600
C	-3.6914222	1.4380840	0.4866984
C	-3.6053082	-0.0058700	0.2755671
N	-4.7952369	-0.6512690	-0.0380528
C	-5.9547898	-0.0249680	-0.0639910
H	-8.7579216	5.0832653	-0.6838877
H	-6.6228244	3.8631485	-0.7861515
H	-8.5777881	0.6057371	1.2302469
H	-10.6367654	1.9477389	1.1992961
H	-4.9599458	3.1373241	0.6529100
C	-2.5143925	2.1775163	0.7599511
O	-2.5393153	-0.6302682	0.3551825
C	-7.1222180	-0.8976731	-0.4734505
H	-6.7473378	-1.6924454	-1.1168911
H	-7.5799531	-1.3748141	0.3984747
H	-7.9004297	-0.3421265	-0.9970060
N	-1.5715657	2.8117978	0.9766744
O	-12.3772146	4.8576173	0.1832971
H	-11.4745901	4.4759375	0.2677635
H	-12.6923414	4.5222697	-0.6616593
O	-3.4221013	-3.3359641	-0.2155146
H	-4.1937307	-2.7487653	-0.2591390
H	-2.7511969	-2.6667032	-0.0003414
O	0.9290377	4.3634999	0.9072039
H	0.0706250	3.9258417	1.0528510
H	1.3475624	3.8088359	0.2413551

ANION-3H₂O (Isomer II)

S₀ state

33

C	-9.6198551	2.5497720	-0.6974344
C	-8.4432328	1.8200581	-0.7334001
C	-7.4291726	2.0624615	0.2107063
C	-7.7078546	3.0811806	1.1421362
C	-8.9124340	3.7617473	1.0960921
N	-9.8742515	3.5117089	0.1981077
C	-6.1455217	1.3519653	0.2205830
C	-4.9706654	2.0667005	0.4857786
C	-3.7316839	1.4547283	0.4763267
C	-3.6196181	0.0268128	0.1818261
N	-4.8156202	-0.6549627	-0.0091533
C	-5.9855609	-0.0483240	-0.0044051
H	-10.3986917	2.3667576	-1.4315503
H	-8.3047254	1.0842988	-1.5129302
H	-6.9919922	3.3212789	1.9181656
H	-9.1290012	4.5420471	1.8193202
H	-5.0242779	3.1341894	0.6689159
C	-2.5582007	2.2123320	0.7111536
O	-2.5312714	-0.5588249	0.1143312
C	-7.1681136	-0.9753552	-0.1912348
H	-6.8966767	-1.9609420	0.1844407
H	-8.0630030	-0.6240048	0.3225111
H	-7.4134196	-1.0878912	-1.2518843
N	-1.6176738	2.8570307	0.9058897
O	-12.4119648	4.8562918	0.1528009
H	-11.5155992	4.4513739	0.1335636
H	-12.8835086	4.3486870	0.8203145
O	-3.4569174	-3.2918191	-0.3648068
H	-4.2172040	-2.6881588	-0.3222103
H	-2.7535516	-2.6392103	-0.2153569
O	0.9320497	4.3468305	0.9172873
H	0.0435050	3.9541017	0.9909976
H	1.4444942	3.6535928	0.4898110

ANION-3H₂O

TICT state

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C	-9.1171948	3.4431883	-0.9508035
C	-7.8835511	2.8462780	-0.9640819
C	-7.3768802	2.2242678	0.2178786
C	-8.2341834	2.2740616	1.3590409
C	-9.4530311	2.8952875	1.2753258
N	-9.9510126	3.5001355	0.1430399
C	-6.0536893	1.5530752	0.2512732
C	-4.9009116	2.2444788	0.5910970
C	-3.6648745	1.6009471	0.6135679
C	-3.5837263	0.1816408	0.2769238
N	-4.7502602	-0.4865559	-0.0552409
C	-5.9005028	0.1443318	-0.0704541
H	-9.4933722	3.9238860	-1.8487053
H	-7.3001160	2.8632121	-1.8786373
H	-7.9321564	1.8325045	2.3029522
H	-10.0969224	2.9399135	2.1483426
H	-4.9725583	3.2955216	0.8377310
C	-2.4769751	2.2933045	0.9501171
O	-2.5011116	-0.4210974	0.2839768
C	-7.1168097	-0.6507816	-0.4424675
H	-6.8372551	-1.6779765	-0.6670577
H	-7.8454733	-0.6304997	0.3701421
H	-7.6158663	-0.2010324	-1.3025528
N	-1.5197552	2.8795504	1.2231798
O	-12.4808574	4.6071786	0.0597717
H	-11.5351048	4.2802370	0.1075026
H	-12.9700940	3.8135327	-0.1775018
O	-3.8314794	-3.2818210	-0.5461943
H	-4.2686889	-2.4202118	-0.4193305
H	-2.9091981	-3.0643576	-0.3725410
O	1.2532471	4.0855689	1.3816797
H	0.3197565	3.8289372	1.4395866
H	1.6563320	3.3648297	0.8872086

CATION-3H₂O (Isomer I)

S₀ state

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C	-1.5994824	2.8524756	-0.6098244
C	-0.5064822	2.0236638	-0.6039145
C	-0.6101628	0.6978740	-0.1231880
C	-1.8759041	0.2989834	0.3572490
C	-2.9396980	1.1665966	0.3311660
N	-2.7916494	2.4161453	-0.1518319
C	0.5647176	-0.1733717	-0.0924130
C	1.8158630	0.4162199	0.1537431
C	2.9596577	-0.3536098	0.2303909
C	2.8225891	-1.7555149	0.0628439
N	1.6485993	-2.3108781	-0.2319006
C	0.5416317	-1.5751904	-0.3174029
H	-1.5684070	3.8674833	-0.9804003
H	0.4308766	2.4030610	-0.9867920
H	-2.0246946	-0.6801405	0.7847835
H	-3.9226164	0.9067025	0.6985767
H	1.9115065	1.4844025	0.3094721
C	4.2202778	0.2644538	0.4689105
O	3.8873535	-2.5096444	0.1897124
C	-0.6825171	-2.3465521	-0.7346275
H	-0.3688199	-3.1829805	-1.3567189
H	-1.1909557	-2.7711450	0.1366447
H	-1.3983610	-1.7423745	-1.2906197
N	5.2033648	0.8425480	0.6434335
H	3.6788107	-3.4761738	0.0633900
O	-5.0116473	4.1065454	-0.1588660
H	-5.2976579	4.6803995	0.5618381
H	-3.6063425	3.0526733	-0.1639380
O	3.5349845	-5.1376417	-0.0609274
H	2.8032148	-5.5447039	-0.5369660
H	4.2840108	-5.7418918	-0.1153376
O	3.1250931	3.3480640	0.1139598
H	3.2436561	4.2635283	0.3896283
H	4.0062405	2.9526533	0.1722256
H	-5.6385321	4.2412730	-0.8796808

CATION-3H₂O (Isomer II)

S₀ state

35

C	-3.1048783	1.2749120	-1.1041095
C	-2.0096965	0.4467596	-1.0898921
C	-0.9297122	0.6976126	-0.2167440
C	-1.0406720	1.8368911	0.6131275
C	-2.1567555	2.6327010	0.5634970
N	-3.1663730	2.3423185	-0.2835520
C	0.2782787	-0.1275876	-0.1808165
C	1.5058074	0.5147869	0.0516728
C	2.6867159	-0.2006794	0.0754383
C	2.6140571	-1.5999309	-0.1456770
N	1.4482925	-2.2189073	-0.3225476
C	0.3035349	-1.5380697	-0.3410727
H	-3.9471270	1.1283704	-1.7656986
H	-1.9821432	-0.3766019	-1.7862365
H	-0.2550130	2.0934919	1.3099086
H	-2.2881461	3.5047058	1.1887118
H	1.5598325	1.5881981	0.1931702
C	3.9202353	0.4677716	0.3199123
O	3.7284309	-2.2903513	-0.1641224
C	-0.9252869	-2.3980842	-0.4749722
H	-1.1740685	-2.5608757	-1.5284493
H	-0.7125822	-3.3748399	-0.0441599
H	-1.7972762	-1.9751091	0.0224754
N	4.8736755	1.0790034	0.5398086
H	3.5640801	-3.2644587	-0.2934482
H	-3.9990405	2.9546196	-0.3121933
O	-5.4141066	3.9924186	-0.4035727
H	-6.2312281	3.9050387	0.1016146
H	-5.5160163	4.7797881	-0.9514526
O	3.5237190	-4.9316057	-0.4397711
H	2.7703654	-5.4057783	-0.8072825
H	4.2992552	-5.4932253	-0.5489867
O	2.5996964	3.4024633	0.9540537
H	3.4912315	3.0405077	1.0552541
H	2.7269534	4.3488778	0.8268353

CATION-3H₂O

TICT state

35

C	-2.1326339	2.1506375	-1.4232256
C	-1.0285158	1.3526962	-1.3975004
C	-0.6059955	0.7363633	-0.1923154
C	-1.3640604	0.9993407	0.9776277
C	-2.4653116	1.7996579	0.9306364
N	-2.8634225	2.3746487	-0.2663336
C	0.6317042	-0.0999443	-0.1345730
C	1.8582701	0.4760439	0.1265605
C	3.0006811	-0.3299727	0.2007139
C	2.8353233	-1.7545087	0.0005851
N	1.6512611	-2.3162611	-0.2699026
C	0.5818768	-1.5418388	-0.3441048
H	-2.4884098	2.6394195	-2.3163635
H	-0.4815367	1.2099751	-2.3198804
H	-1.0825600	0.5758163	1.9324907
H	-3.0701165	2.0250858	1.7947197
H	1.9686614	1.5446329	0.2752618
C	4.2756725	0.2049917	0.4703186
O	3.8897534	-2.4935762	0.0910977
C	-0.7142378	-2.2055671	-0.6560619
H	-0.5678451	-3.2737298	-0.7898291
H	-1.4365414	-2.0271219	0.1440458
H	-1.1559226	-1.7746539	-1.5577419
N	5.3149276	0.6618668	0.6941043
H	3.6991183	-3.4899187	-0.0485611
O	-5.1854909	4.1397265	-0.3047207
H	-5.1959403	5.0886753	-0.1380122
H	-3.6751985	2.9857009	-0.2888628
O	3.5574026	-5.0134456	-0.1904347
H	2.7432749	-5.4397400	-0.4802870
H	4.2760310	-5.6534281	-0.2511631
O	3.1991140	3.3076798	0.4737696
H	2.9127011	4.2250910	0.4070233
H	4.1402013	3.3456785	0.6808643
H	-6.0986254	3.8901403	-0.4842576

Table S3. Cartesian coordinates of the optimized geometric conformations of the hydrogen-bonded complexes for various forms of MIR with the consideration of COSMO solvation model.

KETO-3H₂O_COSMO (Isomer I)

S₀ state

34

C	-8.6677167	3.9102974	-0.6965133
C	-7.4578904	3.2336036	-0.6544566
C	-7.3423760	2.0871737	0.1359223
C	-8.4694151	1.6885164	0.8577094
C	-9.6392162	2.4268087	0.7515788
N	-9.7480201	3.5196136	-0.0115291
C	-6.0513581	1.3598589	0.2246173
C	-4.8831674	2.0709212	0.5473857
C	-3.6523889	1.4568428	0.6519475
C	-3.5161379	0.0390181	0.4231935
N	-4.7143281	-0.5834460	0.0928271
C	-5.9328312	-0.0031584	-0.0154058
H	-8.7790055	4.7962430	-1.3090925
H	-6.6245524	3.5908420	-1.2431211
H	-8.4406743	0.8280227	1.5101782
H	-10.5221202	2.1341767	1.3060694
H	-4.9514218	3.1342919	0.7327185
C	-2.4889221	2.1956608	0.9805924
O	-2.4672713	-0.6141261	0.4909367
H	-4.6194676	-1.5876988	-0.0952070
C	-7.0502951	-0.9163889	-0.4115686
H	-7.8482967	-0.3724540	-0.9078839
H	-7.4700186	-1.4069632	0.4690426
H	-6.6852674	-1.6940611	-1.0812400
N	-1.5442145	2.8028756	1.2432666
O	-12.2033459	4.9211301	-0.3525800
H	-11.3575588	4.4328962	-0.2216906
H	-12.6358604	4.4780016	-1.0905476
O	0.8156445	4.5782704	1.5206712
H	0.0554998	3.9796778	1.4326546
H	1.3934412	4.3566232	0.7820377
O	-3.5038103	-3.1740546	-0.1216824
H	-3.2700454	-3.5970768	-0.9565117
H	-2.8048180	-2.5166647	0.0482400

KETO-3H₂O_COSMO (Isomer I)

S₁ state

34

C	-8.6764379	3.8847232	-0.5845342
C	-7.4348355	3.2734601	-0.5655288
C	-7.2872796	2.0291013	0.0708575
C	-8.4339729	1.4760269	0.6635927
C	-9.6306421	2.1709412	0.6033469
N	-9.7628975	3.3535306	-0.0099335
C	-5.9705253	1.3887607	0.1500295
C	-4.8562856	2.2070065	0.3977081
C	-3.5642671	1.6155071	0.5616181
C	-3.4310924	0.1970204	0.4832901
N	-4.5611550	-0.5410367	0.2174503
C	-5.8132656	-0.0205767	-0.0011202
H	-8.8096922	4.8397748	-1.0767616
H	-6.5973505	3.7462072	-1.0564609
H	-8.3912799	0.5405177	1.1996294
H	-10.5200514	1.7683773	1.0712929
H	-4.9790132	3.2657363	0.5544369
C	-2.4252571	2.3733895	0.8545519
O	-2.3498660	-0.4228587	0.6366397
H	-4.4085974	-1.5553180	0.1195908
C	-6.8485495	-1.0015235	-0.4321845
H	-7.7087536	-0.5151281	-0.8794984
H	-7.1999325	-1.6154911	0.4056739
H	-6.4301963	-1.6874790	-1.1729392
N	-1.4949718	3.0296718	1.0874899
O	-12.1885512	4.8591826	0.0226249
H	-11.3639726	4.3226663	0.0008952
H	-12.6470991	4.6470006	-0.7975276
O	0.8933110	4.6620494	1.5441926
H	0.0936783	4.1268508	1.3939821
H	1.6278217	4.0643984	1.3657851
O	-4.0121998	-3.3463378	0.0266545
H	-4.3742398	-3.9038907	-0.6726270
H	-3.0613119	-3.5104900	0.0094880

KETO-3H₂O_COSMO (Isomer II)

S₀ state

34

C	-9.3703615	2.6946622	-1.0243294
C	-8.1859778	1.9732023	-0.9917676
C	-7.3641475	2.0607125	0.1339329
C	-7.7867447	2.8914591	1.1749512
C	-8.9864055	3.5769880	1.0532205
N	-9.7735318	3.4855817	-0.0242412
C	-6.0666218	1.3441718	0.2217218
C	-4.9003434	2.0697780	0.5186162
C	-3.6606263	1.4702613	0.6023593
C	-3.5157037	0.0496247	0.3981141
N	-4.7184882	-0.5938286	0.1311482
C	-5.9440510	-0.0266505	0.0344004
H	-10.0185807	2.6431807	-1.8902405
H	-7.9070465	1.3700158	-1.8434495
H	-7.1998464	2.9964559	2.0766598
H	-9.3335108	4.2204066	1.8520160
H	-4.9731210	3.1378900	0.6717541
C	-2.4946910	2.2260601	0.8804957
O	-2.4586485	-0.5915663	0.4513683
H	-4.6258035	-1.6088978	0.0117958
C	-7.0694669	-0.9682519	-0.2588537
H	-8.0136935	-0.5855373	0.1168669
H	-6.8786112	-1.9406390	0.1930939
H	-7.1672672	-1.1162070	-1.3363222
N	-1.5471288	2.8448853	1.1025157
O	-12.2369007	4.8880921	-0.2834813
H	-11.3855427	4.4032300	-0.1779102
H	-12.9215000	4.2237904	-0.1493981
O	0.7223469	4.7074337	1.5201298
H	0.0074635	4.0643717	1.3820574
H	1.5305403	4.2364968	1.2893833
O	-3.5083565	-3.1914947	0.0690236
H	-3.3101777	-3.6707750	-0.7441042
H	-2.8041241	-2.5245300	0.1626270

KETO-3H₂O_COSMO (Isomer II)

S₁ state

34

C	-9.3916434	2.3511304	-0.9752758
C	-8.1900009	1.6705213	-0.8687864
C	-7.3088468	1.9911975	0.1762263
C	-7.7180375	2.9964129	1.0689449
C	-8.9439461	3.6126311	0.8855800
N	-9.7747151	3.3058105	-0.1185054
C	-5.9892499	1.3658545	0.3159320
C	-4.9063382	2.1913932	0.6583887
C	-3.5890126	1.6394407	0.7347727
C	-3.3920839	0.2606611	0.4244723
N	-4.4990794	-0.4923802	0.1095266
C	-5.7925212	-0.0296529	0.0936757
H	-10.0759508	2.1275994	-1.7834502
H	-7.9296927	0.9334577	-1.6126508
H	-7.0966690	3.2787556	1.9058435
H	-9.2744300	4.3862108	1.5671515
H	-5.0446179	3.2530234	0.7788360
C	-2.4693309	2.4170818	1.0501389
O	-2.2747668	-0.3126950	0.4249784
H	-4.3147562	-1.4900893	-0.0731329
C	-6.8405987	-1.0716703	-0.0968740
H	-7.8298336	-0.7060203	0.1564304
H	-6.6304109	-1.9359361	0.5390708
H	-6.8651780	-1.4352621	-1.1312274
N	-1.5603279	3.0865011	1.3253527
O	-12.1912774	4.7506188	-0.6311743
H	-11.3726626	4.2434524	-0.4304568
H	-12.9138203	4.1942833	-0.3219885
O	0.8332342	4.7373489	1.6561192
H	0.0311712	4.1954314	1.5508365
H	1.5495664	4.1838426	1.3265076
O	-3.8919676	-3.2511292	-0.3578862
H	-4.3851971	-3.7599494	-1.0128794
H	-2.9637296	-3.3779048	-0.5895567

ENOL-3H₂O_COSMO (Isomer I)

S₀ state

34

C	-2.5064518	2.3236262	-1.0402206
C	-1.2785471	1.6796430	-1.0177749
C	-1.0893556	0.5974861	-0.1548937
C	-2.1665931	0.2201580	0.6500763
C	-3.3592901	0.9226288	0.5590027
N	-3.5356753	1.9588968	-0.2683425
C	0.2284772	-0.0838885	-0.0780211
C	1.3677746	0.6769918	0.1654079
C	2.6168354	0.0717526	0.2623963
C	2.6829828	-1.3280636	0.1071939
N	1.6017452	-2.0500286	-0.1558297
C	0.3961389	-1.4713287	-0.2572149
H	-2.6746936	3.1609412	-1.7064169
H	-0.4867328	2.0132244	-1.6737191
H	-2.0802740	-0.5961763	1.3524741
H	-4.2053084	0.6494220	1.1776885
H	1.2900459	1.7473505	0.2942906
C	3.7888240	0.8293977	0.5159683
O	3.8637833	-1.9316500	0.2189513
C	-0.7339580	-2.4001519	-0.5963464
H	-0.3665421	-3.1971647	-1.2398304
H	-1.1291642	-2.8658961	0.3096537
H	-1.5530421	-1.8857480	-1.0919164
N	4.7367680	1.4533077	0.7203657
H	3.7517974	-2.9135255	0.0876362
O	-5.9147547	3.4826299	-0.4699234
H	-6.3885673	3.1105124	-1.2215960
H	-5.0998057	2.9338047	-0.3848674
O	3.1261109	-4.4841984	-0.1000402
H	2.2584710	-4.0817405	-0.2833843
H	3.3671546	-4.9782221	-0.8934284
O	7.0692876	3.2908047	0.8919967
H	7.8357380	2.7894220	0.5925713
H	6.3267271	2.6666735	0.8449358

ENOL-3H₂O_COSMO (Isomer I)

S₁ state

34

C	-2.4725094	2.4495831	-0.7974193
C	-1.2335605	1.8364268	-0.8027830
C	-1.0834267	0.5553764	-0.2190655
C	-2.2365064	-0.0005214	0.3793228
C	-3.4257254	0.7024102	0.3500193
N	-3.5578439	1.9052463	-0.2313023
C	0.2107072	-0.0968169	-0.2008671
C	1.3672986	0.7389994	-0.1038084
C	2.6369926	0.1289177	0.0494593
C	2.6579680	-1.3076051	0.0701393
N	1.5956685	-2.0811877	-0.1092445
C	0.3650605	-1.5177398	-0.2675746
H	-2.6049639	3.4200339	-1.2586089
H	-0.3988298	2.3230755	-1.2825852
H	-2.1940917	-0.9460471	0.8951958
H	-4.3129329	0.2947881	0.8166144
H	1.2686165	1.8042069	0.0202860
C	3.8086561	0.8550209	0.2720938
O	3.8261006	-1.8835472	0.2824698
C	-0.7116297	-2.4910309	-0.6329447
H	-0.3069267	-3.2166923	-1.3415561
H	-1.0410571	-3.0635711	0.2423488
H	-1.5804549	-2.0235141	-1.0851909
N	4.7714105	1.4877387	0.4450138
H	3.7169106	-2.8902131	0.2788289
O	-5.9968593	3.4305914	-0.2340493
H	-6.3189125	3.4185223	-1.1418378
H	-5.1786211	2.8878275	-0.2433447
O	3.1965326	-4.4197938	0.2513121
H	2.3053312	-4.1184511	-0.0030429
H	3.5090800	-4.9871795	-0.4648527
O	7.0660943	3.2366677	0.8721876
H	7.8128943	2.6446880	1.0128713
H	6.3033565	2.6472603	0.7289462

ENOL-3H₂O_COSMO (Isomer II)

S₀ state

34

C	-3.0823926	1.1353401	-1.3855053
C	-1.8791119	0.4511849	-1.3031609
C	-1.0952080	0.5833266	-0.1552720
C	-1.5786114	1.4103401	0.8612180
C	-2.7964281	2.0545274	0.6918153
N	-3.5433812	1.9261016	-0.4099531
C	0.2268323	-0.0850985	-0.0343348
C	1.3588003	0.6892475	0.1960731
C	2.6163631	0.0977845	0.2762916
C	2.6958555	-1.3008223	0.1206838
N	1.6124032	-2.0439563	-0.0645506
C	0.3988522	-1.4792181	-0.1425692
H	-3.6990885	1.0530319	-2.2719833
H	-1.5543147	-0.1574729	-2.1343059
H	-1.0239436	1.5471446	1.7787689
H	-3.1898392	2.6968214	1.4700236
H	1.2720241	1.7617978	0.2975035
C	3.7896578	0.8658473	0.4859920
O	3.8910234	-1.8841465	0.1724210
C	-0.7458966	-2.4321472	-0.3312790
H	-0.9160561	-2.6172527	-1.3946476
H	-0.5049886	-3.3858448	0.1339975
H	-1.6708823	-2.0484264	0.0921726
N	4.7454560	1.4897857	0.6489438
H	3.7892098	-2.8678425	0.0520273
O	-5.9917828	3.2929056	-0.9181839
H	-6.6715158	2.6103763	-0.9093707
H	-5.1517301	2.8214014	-0.7118093
O	3.1798044	-4.4523482	-0.1126195
H	2.2980397	-4.0627332	-0.2504530
H	3.3879838	-4.9445680	-0.9162222
O	7.0499249	3.3361980	0.9457892
H	7.8486979	2.7993930	0.9915762
H	6.3224092	2.6988463	0.8567968

ENOL-3H₂O_COSMO (Isomer II)

S₁ state

34

C	-3.1976968	0.8297149	-1.2257806
C	-2.0231989	0.1192619	-1.0684531
C	-1.0922076	0.5213931	-0.0846737
C	-1.4370509	1.6598971	0.6817978
C	-2.6498730	2.2871482	0.4640431
N	-3.5218015	1.8930437	-0.4740484
C	0.1847502	-0.1386079	0.0999426
C	1.3034106	0.6796488	0.4500582
C	2.5952119	0.0973499	0.4534321
C	2.6661463	-1.3026231	0.1321843
N	1.6156055	-2.0819392	-0.0854512
C	0.3629773	-1.5456585	-0.0874922
H	-3.9108660	0.5464484	-1.9892126
H	-1.8109424	-0.7063938	-1.7282818
H	-0.7793356	2.0230777	1.4564413
H	-2.9364035	3.1457264	1.0575692
H	1.1993940	1.7486792	0.5311616
C	3.7630344	0.8372652	0.6493594
O	3.8710792	-1.8351964	0.0540428
C	-0.7406772	-2.5530931	-0.1675495
H	-0.8373033	-2.9573251	-1.1822420
H	-0.4963945	-3.3994628	0.4784509
H	-1.7046120	-2.1599751	0.1399035
N	4.7195824	1.4760656	0.8351633
H	3.7971019	-2.8140197	-0.1956191
O	-5.9521020	3.2975254	-1.1023511
H	-6.6720344	2.6922046	-0.8949595
H	-5.1322395	2.8167643	-0.8556094
O	3.3250176	-4.3294497	-0.4988672
H	2.3955455	-4.0380265	-0.5320630
H	3.5254674	-4.7030395	-1.3664008
O	7.0337196	3.2556282	0.8847454
H	7.7880530	2.7006638	1.1106785
H	6.2699805	2.6504671	0.8743590

ANION-3H₂O_COSMO (Isomer I)

S₀ state

33

C	-8.7384442	4.0171802	-0.3595221
C	-7.5206286	3.3577315	-0.3902193
C	-7.3945574	2.0962980	0.2083610
C	-8.5424867	1.5811193	0.8238186
C	-9.7228808	2.3066302	0.7957263
N	-9.8347055	3.5077459	0.2155517
C	-6.0985521	1.3844555	0.2084839
C	-4.9318419	2.0949455	0.4803860
C	-3.6962554	1.4623104	0.5075464
C	-3.6058229	0.0377822	0.2694118
N	-4.7708952	-0.6132386	-0.0535325
C	-5.9466352	0.0032499	-0.0850984
H	-8.8462538	4.9899161	-0.8238204
H	-6.6824536	3.8172144	-0.8951720
H	-8.5220449	0.6309777	1.3360586
H	-10.6178247	1.9145845	1.2632975
H	-4.9839462	3.1549208	0.6916044
C	-2.5155119	2.1879227	0.7810850
O	-2.5172743	-0.5908234	0.3367254
C	-7.1056375	-0.8687387	-0.5021875
H	-6.7364620	-1.6617795	-1.1491151
H	-7.5679011	-1.3414873	0.3678291
H	-7.8780133	-0.3093877	-1.0256729
N	-1.5478036	2.7842710	0.9958725
O	-12.3100170	4.8715161	0.1744158
H	-11.4438027	4.3975495	0.1877677
H	-12.7383014	4.5862903	-0.6399170
O	-3.4352318	-3.1803201	-0.2241227
H	-4.2506103	-2.6514712	-0.2804727
H	-2.8201025	-2.4503003	-0.0121392
O	0.9045047	4.4129973	0.9232081
H	0.1002810	3.8658026	0.9539361
H	1.4513457	4.0128015	0.2382799

ANION-3H₂O_COSMO (Isomer II)

S₀ state

33

C	-9.5895361	2.5826936	-0.7834103
C	-8.4102613	1.8547851	-0.8021699
C	-7.4557762	2.0537275	0.2028972
C	-7.7664235	3.0087216	1.1804118
C	-8.9672949	3.6967997	1.1145104
N	-9.8769254	3.4941332	0.1536618
C	-6.1572616	1.3453296	0.2238647
C	-4.9922649	2.0762461	0.4427364
C	-3.7486784	1.4598348	0.4392673
C	-3.6422042	0.0358931	0.1972565
N	-4.8214740	-0.6551933	0.0418705
C	-6.0066834	-0.0549216	0.0482218
H	-10.3333043	2.4379764	-1.5575962
H	-8.2353328	1.1567617	-1.6073380
H	-7.0848667	3.2070760	1.9959265
H	-9.2174153	4.4360236	1.8658715
H	-5.0490996	3.1457638	0.5975167
C	-2.5674626	2.2065086	0.6403658
O	-2.5374984	-0.5596867	0.1404117
C	-7.1892995	-0.9790876	-0.1040486
H	-6.9290096	-1.9596832	0.2894559
H	-8.0729888	-0.6090953	0.4120338
H	-7.4487253	-1.1055957	-1.1580023
N	-1.5992214	2.8173836	0.8048804
O	-12.3409565	4.8794037	0.2079100
H	-11.4799433	4.3964549	0.1785092
H	-12.8944236	4.3649397	0.8054708
O	-3.5491009	-3.1813783	-0.3843995
H	-4.2824755	-2.5406406	-0.2850610
H	-2.8129022	-2.5621334	-0.2415330
O	0.9114633	4.3207250	0.9022237
H	0.0815482	3.8124619	0.8781772
H	1.5938532	3.6956795	0.6348750

ANION-3H₂O_COSMO

TICT state

33

C	-9.2900637	3.2138095	-1.0014017
C	-8.0188952	2.7104693	-1.0391442
C	-7.4326394	2.1849921	0.1562181
C	-8.2366478	2.2377379	1.3369423
C	-9.4988352	2.7608917	1.2720981
N	-10.0773404	3.2625376	0.1262925
C	-6.0685743	1.6338396	0.1708253
C	-4.9584590	2.4372542	0.4207410
C	-3.6839987	1.8861125	0.4558352
C	-3.4998032	0.4555473	0.2251360
N	-4.6075943	-0.3213694	-0.0360232
C	-5.8099439	0.2152269	-0.0722117
H	-9.7361183	3.6124715	-1.9051203
H	-7.4752103	2.7198731	-1.9757244
H	-7.8655968	1.8726192	2.2868837
H	-10.1112611	2.7992841	2.1650295
H	-5.1038873	3.4932967	0.5944235
C	-2.5385524	2.6736721	0.7223006
O	-2.3675528	-0.0617644	0.2601354
C	-6.9659938	-0.6832019	-0.3584744
H	-6.6238881	-1.6871989	-0.5944643
H	-7.6333515	-0.7126634	0.5044898
H	-7.5620748	-0.2827954	-1.1777965
N	-1.6064474	3.3189698	0.9426098
O	-12.7324956	3.5548969	-0.1033745
H	-11.7229221	3.4885078	-0.0004370
H	-12.9992159	2.6658098	-0.3597342
O	-3.9445596	-3.1000685	-0.7361503
H	-4.2068532	-2.2010700	-0.4536200
H	-4.6648659	-3.6799914	-0.4660763
O	1.2574441	3.6683868	1.8993827
H	0.3412138	3.7755115	1.6071689
H	1.5489224	4.5529859	2.1479299

CATION-3H₂O_COSMO (Isomer I)

S₀ state

35

C	-1.6784595	2.7363708	-0.7302438
C	-0.5642571	1.9307869	-0.7501653
C	-0.5897995	0.6796673	-0.1162502
C	-1.7750152	0.3008242	0.5298467
C	-2.8636224	1.1413640	0.5207165
N	-2.7941068	2.3275381	-0.1044610
C	0.6168749	-0.1714446	-0.0923741
C	1.8478419	0.4252837	0.1792015
C	2.9974126	-0.3478439	0.2711675
C	2.8703136	-1.7425037	0.0875032
N	1.7119633	-2.3007871	-0.2339613
C	0.6009394	-1.5631881	-0.3352467
H	-1.7176928	3.7033116	-1.2058822
H	0.3159142	2.2738950	-1.2716562
H	-1.8495596	-0.6332364	1.0624265
H	-3.7969810	0.9038313	1.0059829
H	1.9300528	1.4933163	0.3349027
C	4.2568981	0.2385113	0.5637064
O	3.9438766	-2.5065878	0.2291206
C	-0.6259374	-2.3186381	-0.7632719
H	-0.3272022	-3.1370739	-1.4145291
H	-1.1264439	-2.7584875	0.1023648
H	-1.3423985	-1.6891099	-1.2849341
N	5.2753752	0.7258512	0.8015537
H	3.7107419	-3.4715370	0.1053321
O	-5.0255959	3.9396317	-0.0792992
H	-5.0120666	4.7262914	0.4794924
H	-3.6277660	2.9507122	-0.1032442
O	3.3688275	-5.0922971	0.0327536
H	2.5601341	-5.2333825	-0.4749263
H	4.0264323	-5.6872603	-0.3487487
O	3.2205731	3.3948260	0.1280696
H	3.0842987	4.3260577	0.3386893
H	4.1180446	3.2069092	0.4273704
H	-5.3964725	4.2257346	-0.9226373

CATION-3H₂O_COSMO (Isomer II)

S₀ state

35

C	-3.0085162	1.3547624	-1.2309235
C	-1.9046981	0.5353381	-1.1853889
C	-0.9383663	0.7157735	-0.1859443
C	-1.1438342	1.7481111	0.7413757
C	-2.2636174	2.5413676	0.6529462
N	-3.1636892	2.3291287	-0.3204226
C	0.2880922	-0.1059409	-0.1267580
C	1.5102607	0.5369013	0.0671897
C	2.6915960	-0.1923864	0.0807508
C	2.6065071	-1.5908028	-0.0992792
N	1.4410204	-2.2072647	-0.2331978
C	0.2974156	-1.5133278	-0.2483106
H	-3.7771041	1.2688100	-1.9824224
H	-1.7914372	-0.2202887	-1.9455003
H	-0.4407843	1.9272823	1.5400644
H	-2.4750360	3.3439918	1.3415168
H	1.5644714	1.6106581	0.1964347
C	3.9467947	0.4477443	0.2558469
O	3.7253978	-2.3004286	-0.1205112
C	-0.9494567	-2.3450753	-0.3589857
H	-1.1957066	-2.5282028	-1.4076275
H	-0.7720159	-3.3121025	0.1059599
H	-1.8085838	-1.8731161	0.1114948
N	4.9601937	0.9814086	0.3965540
H	3.5320575	-3.2747606	-0.2390044
H	-4.0055805	2.9392128	-0.3756353
O	-5.4121919	3.8903523	-0.5697076
H	-6.1126088	3.8149434	0.0897457
H	-5.3063620	4.8361069	-0.7294381
O	3.3603780	-4.9204360	-0.3679926
H	2.5461861	-5.1647089	-0.8251975
H	4.0665728	-5.3994290	-0.8200855
O	2.6471958	3.4967649	1.0242423
H	3.5889019	3.3326982	0.8947432
H	2.5003819	4.3756093	0.6552463

CATION-3H₂O_COSMO

TICT state

35

C	-1.9779965	2.1233972	-1.6443850
C	-0.8848988	1.3181725	-1.5686887
C	-0.4827213	0.7750493	-0.3163175
C	-1.2370495	1.1215200	0.8391665
C	-2.3250323	1.9287380	0.7255152
N	-2.7051031	2.4237097	-0.5079817
C	0.7208700	-0.0749225	-0.2090353
C	1.9808328	0.4832349	0.0108790
C	3.0915996	-0.3409481	0.1045680
C	2.8978721	-1.7687310	-0.0208364
N	1.6987124	-2.3191093	-0.2298576
C	0.6377448	-1.5331077	-0.3280207
H	-2.3240447	2.5586107	-2.5670385
H	-0.3364256	1.1065533	-2.4750796
H	-0.9657676	0.7556279	1.8188300
H	-2.9309565	2.2178028	1.5681250
H	2.0983691	1.5571972	0.1146390
C	4.3969031	0.1644544	0.3236760
O	3.9389824	-2.5302018	0.0795504
C	-0.6761019	-2.1759971	-0.5629071
H	-0.5676908	-3.2535701	-0.6356357
H	-1.3663451	-1.9168984	0.2425856
H	-1.1319602	-1.7747963	-1.4700258
N	5.4650547	0.5627338	0.5007411
H	3.7019193	-3.5530991	0.0104354
O	-5.1742417	4.0559822	-0.3112734
H	-5.0690064	4.6719900	0.4236646
H	-3.5255423	3.0195930	-0.5674792
O	3.4351187	-4.9807198	0.0425156
H	2.5957056	-5.2436116	-0.3570233
H	4.1065294	-5.5849889	-0.3013147
O	2.8718898	3.5217594	0.5642707
H	2.2986933	3.8515744	1.2677284
H	2.6580493	4.0798612	-0.1940770
H	-5.8830391	3.4620190	-0.0361227