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Supplementary Material: Exploring ground-state and ionization potentials of the $H_2CO\cdots HNO$ dimers

Gabriel L. C. de Souza*[a,b] and Kirk A. Peterson*[c]

[a] *Centro de Ciências da Natureza, Universidade Federal de São Carlos, Buri, São Paulo, 18290-000 Brazil; E-mail: gabriellcs@ufscar.br*

[b] *Instituto de Física, Universidade Federal de Mato Grosso, Cuiabá, Mato Grosso, 78060-900 Brazil.*

[c] *Department of Chemistry, Washington State University, Pullman, Washington, 99164 USA. E-mail: kipeters@wsu.edu*

Table S1 Vertical ionization potentials (IPs) for the conformation I of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	9.63	9.88	9.96	9.97	10.01
2	11.02	11.25	11.33	11.33	11.37
3	14.71	14.85	14.91	14.90	14.95
4	15.30	15.52	15.60	15.60	15.65
5	16.09	16.20	16.26	16.24	16.30
6	16.21	16.41	16.49	16.49	16.53
7	16.26	16.79	16.95	16.98	17.04
8	17.35	17.51	17.58	17.57	17.61
9	18.13	18.29	18.36	18.35	18.40
10	18.33	18.92	19.07	19.13	19.16
11	19.71	20.32	20.47	20.53	20.56
12	20.11	20.67	20.82	20.87	20.91

Table S2 Core correlation effects for the vertical ionization potentials (IPs) for the conformation I of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	9.64	9.90	0.007	0.03
2	11.03	11.26	0.006	0.02
3	14.72	14.86	0.007	0.02
4	15.32	15.54	0.01	0.03
5	16.10	16.21	0.01	0.02
6	16.24	16.43	0.04	0.03
7	16.27	16.82	0.03	0.14
8	17.35	17.52	0.01	0.02
9	18.14	18.30	0.01	0.03
10	18.35	18.95	0.05	0.12
11	19.73	20.34	0.05	0.12
12	20.14	20.70	0.05	0.11

Table S3 Raw values used for computing the vertical ionization potentials (IPs) for the conformation I of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42862965110479	-244.62126505113588	-244.68074053572940
1, A'	-244.07460754342202	-244.25808606585093	-244.31462271570251
2, A'	-244.02364218041703	-244.20777511893658	-244.26443480542756
3, A"	-243.88795349587872	-244.07550252651191	-244.13264458445855
4, A'	-243.86623285027147	-244.05083768515505	-244.10728271562562
5, A"	-243.83729933612310	-244.02576712074162	-244.08305919344309
6, A'	-243.83112851413065	-244.01811175038131	-244.07474567254329
7, A"	-243.83304527094037	-244.00424844227055	-244.05798714312601
8, A'	-243.79119283319153	-243.97777509373677	-244.03487009983013
9, A'	-243.76252378410143	-243.94918855029255	-244.00606152338810
10, A"	-243.75519810796433	-243.92599256878756	-243.97982024251863
11, A"	-243.70434582765054	-243.87462156707940	-243.92836895563389
12, A"	-243.68945621623519	-243.86150607076999	-243.91546560982727

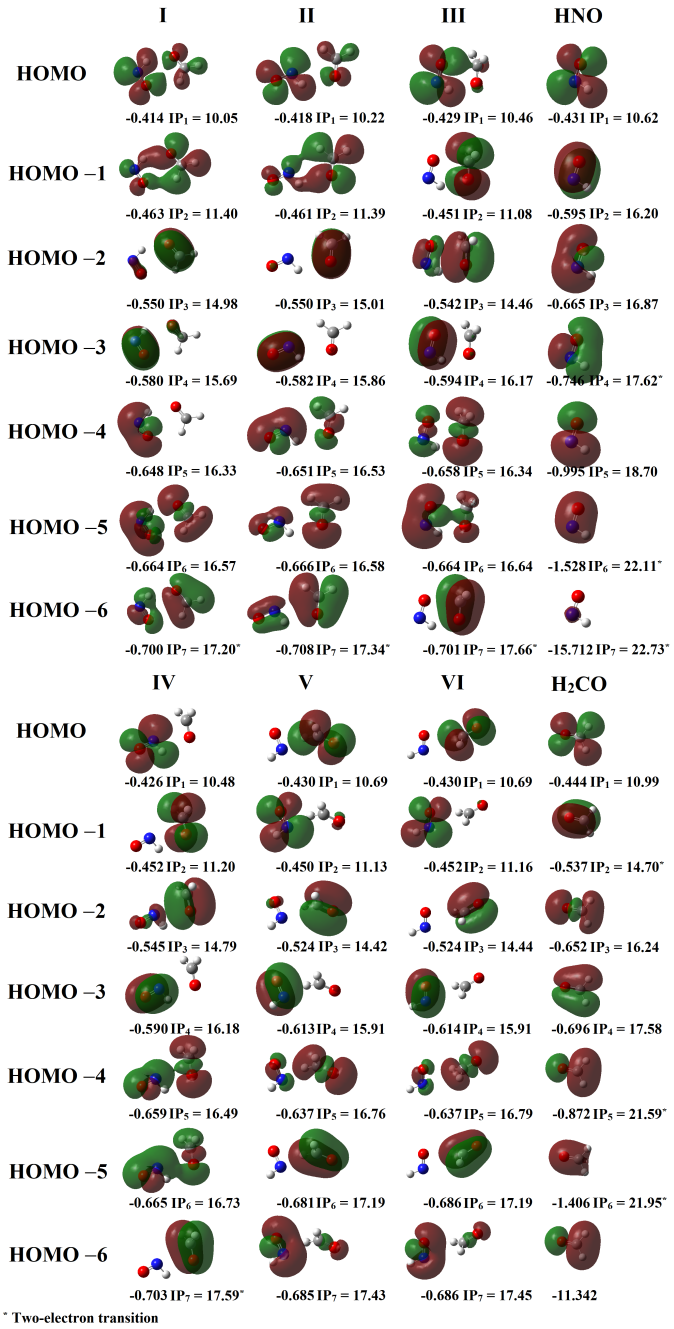

Fig. S1 Molecular orbital plots generated at HF/aug-cc-pVTZ for the six conformations of the $H_2CO\cdots HNO$ dimer, H_2CO, and HNO. The orbital energies are given in hartrees while the corresponding FPD IPs are provided in eV.

Table S4 Raw values used for computing the vertical ionization potentials (IPs) for the conformation I of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	E_{ACVDZ}	E_{ACVTZ}
Ground	-244.58940215650310	-244.83742278828169
1	-244.23477134540991	-244.47266997762230
2	-244.18389609934667	-244.42264976827980
3	-244.04820155553764	-244.29048665539560
4	-244.02618442720200	-244.26535507278751
5	-243.99770467142946	-244.24082796346133
6	-243.99111959800189	-244.23281526047657
7	-243.99041049939481	-244.21424292555858
8	-243.95141847474380	-244.19282802522974
9	-243.92263544008338	-244.16404259965009
10	-243.91301800757020	-244.13683549570786
11	-243.86233304137272	-244.08558333733566
12	-243.84749732644457	-244.07269692209962

Table S5 Raw values used for computing the vertical ionization potentials (IPs) for the conformation I of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}
Ground	-244.43819098711705	-244.63002165101736
1	-244.08381224405554	-244.26638032942739
2	-244.03290291538198	-244.21616002467499
3	-243.89723804956205	-244.08401997572912
4	-243.87534146562493	-244.05913053155945
5	-243.84668291931962	-244.03431283724802
6	-243.84014763732895	-244.02641243533026
7	-243.84149610191679	-244.01191716630450
8	-243.80045641167757	-243.98628950860754
9	-243.77171132620171	-243.95760231142648
10	-243.76380568473635	-243.93381296410840
11	-243.71303380737686	-243.88246781344566
12	-243.69818271612763	-243.86944667031514

Table S6 Vertical ionization potentials (IPs) for the conformation II of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	9.76	10.01	10.09	10.10	10.14
2	10.97	11.20	11.27	11.28	11.32
3	14.70	14.83	14.90	14.88	14.93
4	15.44	15.65	15.74	15.73	15.78
5	16.23	16.36	16.42	16.41	16.45
6	16.26	16.38	16.46	16.42	16.50
7	16.29	16.89	17.04	17.09	17.13
8	17.49	17.65	17.71	17.71	17.75
9	18.08	18.24	18.31	18.29	18.35
10	18.11	18.70	18.86	19.91	19.95
11	19.40	20.00	20.16	20.22	20.26
12	20.15	20.70	20.86	20.90	20.94

Table S7 Core correlation effects for the vertical ionization potentials (IPs) for the conformation II of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (X = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	9.77	10.02	0.007	0.03
2	10.98	11.21	0.006	0.02
3	14.71	14.84	0.007	0.02
4	15.45	15.67	0.01	0.03
5	16.25	16.37	0.01	0.02
6	16.26	16.39	0.002	0.03
7	16.33	16.92	0.07	0.14
8	17.49	17.66	0.01	0.02
9	18.09	18.25	0.01	0.03
10	18.13	18.73	0.05	0.12
11	19.42	20.03	0.05	0.12
12	20.17	20.73	0.05	0.11

Table S8 Raw values used for computing the vertical ionization potentials (IPs) for the conformation II of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42728365558870	-244.61975988514760	-244.67926200550951
1, A'	-244.06854363563670	-244.25189818593805	-244.30843271192541
2, A'	-244.02412480744482	-244.20831934977471	-244.26498970697435
3, A"	-243.88704975206258	-244.07465876274972	-244.13179874590327
4, A'	-243.85998586198593	-244.04450907831560	-244.10095289586661
5, A"	-243.82981386716642	-244.01853495417677	-244.07584777114053
6, A'	-243.83084343452163	-244.01785716651378	-244.07448815660706
7, A"	-243.82853569648049	-243.99924898711728	-244.05295992583299
8, A'	-243.78465185669103	-243.97114243420285	-244.02832553724818
9, A'	-243.76302581305157	-243.94963346378105	-244.00642972904899
10, A"	-243.76193252483625	-243.93241198194599	-243.98610035103471
11, A"	-243.71452726710172	-243.88461875314610	-243.93824825464640
12, A"	-243.68697992916407	-243.85892209857076	-243.91286560082233

Table S9 Raw values used for computing the vertical ionization potentials (IPs) for the conformation II of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	E_{ACVDZ}	E_{ACVTZ}
Ground	-244.58805299445277	-244.83593462935553
1	-244.22870871122421	-244.46649418304816
2	-244.18435647753262	-244.42320390735321
3	-244.04727000988785	-244.28964913685758
4	-244.01993858479145	-244.25903256564109
5	-243.99051104943965	-244.23361971543386
6	-243.99080565645727	-244.23256709605997
7	-243.98562768166255	-244.20925504559301
8	-243.94488469658717	-244.18626985652975
9	-243.92309522874811	-244.16443493744433
10	-243.91981663777423	-244.14328207699893
11	-243.87253284852468	-244.09556400105532
12	-243.84501349541284	-244.07013277983796

Table S10 Raw values used for computing the vertical ionization potentials (IPs) for the conformation II of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}
Ground	-244.43685036507244	-244.62853734371467
1	-244.07775804317384	-244.26020722974582
2	-244.03336955240908	-244.21670725862634
3	-243.89631482936889	-244.08317901476565
4	-243.86910390343061	-244.05281525448532
5	-243.83938583176516	-244.02710444172837
6	-243.83984060137809	-244.02615593618282
7	-243.83682128618315	-244.00692634683151
8	-243.79394327896628	-243.97971300929783
9	-243.77216104288098	-243.95800586362341
10	-243.77057262868018	-243.94023567332334
11	-243.72323218596358	-243.89246343144688
12	-243.69570283417426	-243.86686975768433

Table S11 Vertical ionization potentials (IPs) for the conformation III of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	10.09	10.31	10.39	10.39	10.44
2	10.70	10.93	11.01	11.02	11.06
3	14.16	14.32	14.39	14.38	14.43
4	15.82	16.02	16.10	16.09	16.15
5	16.03	16.19	16.27	16.25	16.31
6	16.42	16.53	16.59	16.57	16.62
7	16.72	17.27	17.42	17.46	17.51
8	17.38	17.54	17.60	17.60	17.64
9	18.21	18.57	18.65	18.70	18.69
10	18.43	18.81	18.96	18.94	19.05
11	19.70	20.30	20.46	20.51	20.54
12	20.37	20.92	21.08	21.12	21.16

Table S12 Core correlation effects for the vertical ionization potentials (IPs) for the conformation III of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (X = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	10.10	10.33	0.007	0.03
2	10.70	10.94	0.006	0.02
3	14.17	14.33	0.008	0.03
4	15.84	16.03	0.009	0.03
5	16.05	16.20	0.01	0.03
6	16.42	16.54	0.01	0.02
7	16.75	17.30	0.06	0.14
8	17.38	17.55	0.01	0.02
9	18.24	18.58	0.05	0.03
10	18.44	18.83	0.01	0.12
11	19.72	20.33	0.05	0.12
12	20.39	20.95	0.05	0.11

Table S13 Raw values used for computing the vertical ionization potentials (IPs) for the conformation III of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42919499844811	-244.62161282491570	-244.68109761611456
1, A'	-244.05849228992642	-244.24256772709450	-244.29920368522593
2, A''	-244.03612306720370	-244.21983532529487	-244.27645106999447
3, A'	-243.90874039200779	-244.09526318611270	-244.15218989999849
4, A'	-243.84765583057842	-244.03289695271098	-244.08945101263976
5, A'	-243.84005130454636	-244.02662621804697	-244.08325074979277
6, A''	-243.82581582754685	-244.01418101467729	-244.07147104223043
7, A''	-243.81479749761894	-243.98705818820298	-244.04095590269898
8, A''	-243.79068988590191	-243.97695185026993	-244.03419705962796
9, A'	-243.75982773063237	-243.93908132033840	-243.99585117289365
10, A'	-243.75199720953194	-243.93054348220863	-243.98441855602709
11, A'	-243.70530165509882	-243.87560026151053	-243.92939270953983
12, A''	-243.68072587042352	-243.85270614542478	-243.90658505140385

Table S14 Raw values used for computing the vertical ionization potentials (IPs) for the conformation III of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
Ground	-244.59009065271121	-244.83772344800272
1	-244.21879390368161	-244.45717213055406
2	-244.19650151246003	-244.43464378772160
3	-244.06905213398286	-244.31006135739835
4	-244.00776912933694	-244.24744716087608
5	-244.00016008822797	-244.24126211651893
6	-243.98629739009576	-244.22920141176905
7	-243.97236696242885	-244.19712874951571
8	-243.95109388150112	-244.19206113395902
9	-243.91779416547564	-244.15382137320472
10	-243.91220079159410	-244.14138854424385
11	-243.86342767675725	-244.08654983539239
12	-243.83886361659981	-244.06384111672631

Table S15 Raw values used for computing the vertical ionization potentials (IPs) for the conformation III of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	$\mathbf{E}^{FC}_{ACVDZ}$	$\mathbf{E}^{FC}_{ACVTZ}$
Ground	-244.43878288693080	-244.63032913925241
1	-244.06772770889322	-244.25083615544594
2	-244.04541684873197	-244.22817733620113
3	-243.91802908625939	-244.10370596634021
4	-243.85680687793649	-244.04117052301496
5	-243.84910004933522	-244.03488763912952
6	-243.83521341104370	-244.02269230142429
7	-243.82330764163984	-243.99471252287131
8	-243.80004242552630	-243.98549767792551
9	-243.76846984714311	-243.94741052665512
10	-243.76118397425165	-243.93833268093420
11	-243.71401823643896	-243.88340558550172
12	-243.68948095970541	-243.86060236739954

Table S16 Vertical ionization potentials (IPs) for the conformation IV of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	10.01	10.25	10.33	10.33	10.37
2	10.75	10.98	11.06	11.06	11.11
3	14.45	14.59	14.66	14.64	14.69
4	15.75	15.95	16.03	16.02	16.08
5	16.12	16.27	16.35	16.32	16.39
6	16.44	16.54	16.60	16.57	16.63
7	16.55	17.11	17.27	17.31	17.36
8	17.43	17.60	17.66	17.65	17.69
9	17.94	18.36	18.43	18.51	18.48
10	18.21	18.54	18.70	18.66	18.79
11	19.28	19.89	20.05	20.10	20.14
12	20.06	20.61	20.77	20.81	20.85

Table S17 Core correlation effects for the vertical ionization potentials (IPs) for the conformation IV of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (X = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	10.02	10.26	0.007	0.03
2	10.76	10.99	0.006	0.02
3	14.46	14.60	0.007	0.03
4	15.76	15.96	0.01	0.03
5	16.13	16.28	0.01	0.03
6	16.44	16.54	0.004	0.02
7	16.58	17.14	0.06	0.14
8	17.44	17.60	0.01	0.02
9	18.96	18.37	0.05	0.03
10	18.22	18.57	0.01	0.12
11	19.30	19.91	0.05	0.12
12	20.08	20.64	0.05	0.11

Table S18 Raw values used for computing the vertical ionization potentials (IPs) for the conformation IV of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (X = D, T, and Q) approaches. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42648223487592	-244.61881418202108	-244.67833547981212
1, A'	-244.05844961328825	-244.24214495950133	-244.29876418654254
2, A"	-244.03125907081380	-244.21522927499899	-244.27187218395321
3, A'	-243.89555045765601	-244.08268830992930	-244.13975315004828
4, A'	-243.84776875207135	-244.03277185228745	-244.08931716411888
5, A'	-243.83414399924251	-244.02100638534634	-244.07765059005209
6, A"	-243.82240520684670	-244.01101949048251	-244.06838077852578
7, A"	-243.81838889178385	-243.98990780910520	-244.04371147532299
8, A"	-243.78579218648343	-243.97221508849103	-244.02947475719029
9, A'	-243.76724821318794	-243.94412833210433	-244.00091418733109
10, A'	-243.75735629615167	-243.93751294623212	-243.99117152027620
11, A'	-243.71807630761197	-243.88806736910865	-243.94169289449252
12, A"	-243.68941928741350	-243.86128700327379	-243.91523452638759

Table S19 Raw values used for computing the vertical ionization potentials (IPs) for the conformation IV of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	E_{ACVDZ}	E_{ACVTZ}
Ground	-244.58728641767459	-244.83497806220137
1	-244.21866661396717	-244.45676731775296
2	-244.19152768904601	-244.43009933457924
3	-244.05576153001326	-244.29759640329272
4	-244.00780055350165	-244.24735463958075
5	-243.99413504962951	-244.23570176055054
6	-243.98292067164479	-244.22611406963392
7	-243.97577039007771	-244.19996005229586
8	-243.94607916662181	-244.18738529694369
9	-243.92519277871136	-244.15889798302976
10	-243.91746367144503	-244.14839640320361
11	-243.87613492250901	-244.09902269799721
12	-243.84750723302403	-244.07253214890565

Table S20 Raw values used for computing the vertical ionization potentials (IPs) for the conformation IV of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}
Ground	-244.43605436891241	-244.62759046870170
1	-244.06767818765374	-244.25045911456459
2	-244.04051174091848	-244.22361164228693
3	-243.90479373075908	-244.09117925707358
4	-243.85692511628150	-244.04110565420510
5	-243.84314197362787	-244.02929998394319
6	-243.83184282096281	-244.01959630535086
7	-243.82683961451585	-243.99759039407266
8	-243.79509758363960	-243.98080137036723
9	-243.77590326571126	-243.95248914132475
10	-243.76649996747364	-243.94533203088218
11	-243.72679185540068	-243.89590582421107
12	-243.69815826945160	-243.86923694811557

Table S21 Vertical ionization potentials (IPs) for the conformation V of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	10.21	10.43	10.51	10.51	10.55
2	10.61	10.86	10.94	10.94	10.98
3	14.05	14.18	14.25	14.23	14.28
4	15.50	15.65	15.73	15.71	15.77
5	16.28	16.49	16.57	16.56	16.62
6	16.81	16.96	17.02	17.01	17.06
7	17.07	17.20	17.26	17.24	17.29
8	17.18	17.75	17.91	17.95	18.00
9	17.57	18.16	18.32	18.37	18.41
10	18.77	18.93	19.01	18.99	19.05
11	18.95	19.56	19.72	19.77	19.81
12	20.32	20.89	21.05	21.09	21.14

Table S22 Core correlation effects for the vertical ionization potentials (IPs) for the conformation V of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (X = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	10.21	10.44	0.005	0.02
2	10.62	10.87	0.007	0.03
3	14.06	14.19	0.006	0.02
4	15.51	15.66	0.006	0.03
5	16.29	16.50	0.01	0.03
6	16.81	16.96	0.01	0.02
7	17.07	17.20	0.01	0.02
8	17.21	17.78	0.06	0.14
9	17.59	18.19	0.05	0.12
10	18.78	18.94	0.01	0.03
11	19.98	19.58	0.05	0.12
12	20.35	20.91	0.05	0.11

Table S23 Raw values used for computing the vertical ionization potentials (IPs) for the conformation V of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (X = D, T, and Q) approach. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42526280305617	-244.61740044450065	-244.67686729926621
1, A"	-244.05019201881495	-244.23394918499335	-244.29062525884314
2, A'	-244.03528281329909	-244.21846786767213	-244.27494799045635
3, A'	-243.90889699590855	-244.09615741695154	-244.15332337569703
4, A'	-243.85582440674312	-244.04225340386355	-244.09889298812595
5, A'	-243.82714554937019	-244.01158083926956	-244.06795746828828
6, A"	-243.80759964102856	-243.99418349166976	-244.05140631415753
7, A"	-243.79798608622269	-243.98550150512116	-244.04274545999860
8, A"	-243.79394362582687	-243.96511137540466	-244.01876971389817
9, A'	-243.77966578088132	-243.94995537849621	-244.00369844240487
10, A'	-243.73547660779036	-243.92167887416051	-243.97829695659379
11, A'	-243.72877770502723	-243.89861438392771	-243.95229534306219
12, A"	-243.67839421522945	-243.84973350494460	-243.90345712600325

Table S24 Raw values used for computing the vertical ionization potentials (IPs) for the conformation V of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	E_{ACVDZ}	E_{ACVTZ}
Ground	-244.58602299515272	-244.83358928394981
1	-244.21044571102047	-244.44890381629943
2	-244.19543760549189	-244.43306127150171
3	-244.06912251507535	-244.31119998465215
4	-244.01580322382415	-244.25699850220758
5	-243.98709016687374	-244.22612341790526
6	-243.96788710988392	-244.20935894101561
7	-243.95838142681265	-244.20064186784637
8	-243.95127432985780	-244.17508977674672
9	-243.93758068481984	-244.16090894018413
10	-243.89551721430269	-244.13640718693716
11	-243.88680885430671	-244.10962307673503
12	-243.83636905446173	-244.06086869720247

Table S25 Raw values used for computing the vertical ionization potentials (IPs) for the conformation V of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}
Ground	-244.43482346617816	-244.62621946888169
1	-244.05944861183119	-244.24238386295204
2	-244.04449199282945	-244.22680908479072
3	-243.91816336830277	-244.10472227454920
4	-243.86484261134513	-244.05059228385093
5	-243.83624457420404	-244.01991739108232
6	-243.81692067478190	-244.00280646170737
7	-243.80737269633315	-243.99412084550292
8	-243.80237773666386	-243.97280610120404
9	-243.78832147418555	-243.95782888876718
10	-243.74459790238922	-243.93006183753377
11	-243.73749469666294	-243.90650214640644
12	-243.68709324187304	-243.85768726659637

Table S26 Vertical ionization potentials (IPs) for the conformation VI of the $H_2CO\cdots HNO$ dimer as computed using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches along with CBS limit extrapolations. All the values are given in eV.

IP	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}	$E_{CBS[DT]}$	$E_{CBS[TQ]}$
1	10.21	10.44	10.51	10.52	10.56
2	10.64	10.88	10.97	10.97	11.01
3	14.07	14.20	14.26	14.25	14.30
4	15.49	15.65	15.72	15.70	15.77
5	16.30	16.51	16.60	16.59	16.65
6	16.81	16.96	17.02	17.02	17.06
7	17.09	17.21	17.28	17.26	17.31
8	17.20	17.78	17.94	17.98	18.03
9	17.57	18.16	18.32	18.37	18.41
10	18.79	18.95	19.03	19.01	19.07
11	18.97	19.57	19.73	19.79	19.82
12	20.35	20.90	21.03	21.09	20.10

Table S27 Core correlation effects for the vertical ionization potentials (IPs) for the conformation VI of the $H_2CO\cdots HNO$ dimer determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IP	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}	Δ_{CV}(DZ)	Δ_{CV}(TZ)
1	10.22	10.45	0.005	0.02
2	10.64	10.89	0.007	0.03
3	14.07	14.21	0.006	0.02
4	15.50	15.66	0.006	0.03
5	16.31	16.52	0.01	0.03
6	16.81	16.96	0.01	0.02
7	17.09	17.22	0.01	0.02
8	17.23	17.80	0.06	0.14
9	17.59	18.18	0.05	0.12
10	18.80	18.96	0.01	0.03
11	18.99	19.59	0.05	0.12
12	20.37	20.91	0.05	0.10

Table S28 Raw values used for computing the vertical ionization potentials (IPs) for the conformation VI of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approach. The values are given in hartrees.

State #, Symmetry	E_{AVDZ}	E_{AVTZ}	E_{AVQZ}
Ground, A'	-244.42513550076757	-244.61728198767474	-244.67672709679655
1, A"	-244.05002280610825	-244.23379848917776	-244.29046227021658
2, A'	-244.03433527946055	-244.21745071956528	-244.27390196649705
3, A'	-243.90820364912457	-244.09550080349604	-244.15266734453908
4, A'	-243.85596172576717	-244.04238255810083	-244.09900139885545
5, A'	-243.82621738875156	-244.01060382592965	-244.06695607287244
6, A"	-243.80752190996623	-243.99405433094725	-244.05126238538460
7, A"	-243.79725344179482	-243.98480287622283	-244.04201810597203
8, A"	-243.79309251244464	-243.96413569433997	-244.01776415001225
9, A'	-243.77970622245101	-243.95005714628900	-244.00380482216249
10, A'	-243.73484452075991	-243.92101000815376	-243.97760256953933
11, A'	-243.72822929340157	-243.89813926838167	-243.95182294665017
12, A'	-243.67736614869114	-243.84947558699204	-243.90410497053654

Table S29 Raw values used for computing the vertical ionization potentials (IPs) for the conformation VI of the $H_2CO\cdots HNO$ dimer as determined using the EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approach with all electrons correlated. The values are given in hartrees.

State #	E_{ACVDZ}	E_{ACVTZ}
Ground	-244.58588376716631	-244.83346220605068
1	-244.21027212117332	-244.44875237625368
2	-244.19447775002746	-244.43202967548609
3	-244.06843080727256	-244.31055162706397
4	-244.01593451954477	-244.25712135073385
5	-243.98614735826249	-244.22513235705935
6	-243.96779748867897	-244.20923135501783
7	-243.95764431100605	-244.19992465725380
8	-243.95040484975019	-244.17409468927036
9	-243.93760741962430	-244.16100882262032
10	-243.89487115017275	-244.13572474218824
11	-243.88625209024340	-244.10915136868326
12	-243.83532798948224	-244.06131501141164

Table S30 Raw values used for computing the vertical ionization potentials (IPs) for the conformation VI of the $H_2CO\cdots HNO$ dimer as determined using the frozen-core EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in hartrees.

State #	E^{FC}_{ACVDZ}	E^{FC}_{ACVTZ}
Ground	-244.43469289891408	-244.62609319770277
1	-244.05928213200198	-244.24222969050683
2	-244.04354232396929	-244.22578324515848
3	-243.91747655704691	-244.10406576896051
4	-243.86498308277069	-244.05071732699582
5	-243.83531090391378	-244.01893019539898
6	-243.81684041718523	-244.00267270545757
7	-243.80664141531076	-243.99341266547546
8	-243.80152065023370	-243.97182046768265
9	-243.78835804196197	-243.95792652492125
10	-243.74396182988247	-243.92938343067675
11	-243.73694387795103	-243.90602331639033
12	-243.68605564637699	-243.85761901482562

Table S31 Cartesian coordinates of the H_2CO molecule as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.0000000000	0.0000000000	-0.0123942092
O	0.0000000000	0.0000000000	1.1951551230
H	0.0000000000	0.9379023863	-0.5913804569
H	0.0000000000	-0.9379023863	-0.5913804569

Table S32 Cartesian coordinates of the HNO molecule as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
H	-0.6680200968	0.6213440334	0.0000000000
N	0.3338048122	0.2947585035	0.0000000000
O	0.3342152846	-0.9161025369	0.0000000000

Table S33 Cartesian coordinates for the conformation I of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
H	-1.5366510800	-1.9374510004	0.0000000000
C	-0.8264447405	-1.0959765361	0.0000000000
H	0.2464067978	-1.3348996381	0.0000000000
O	-1.2160692019	0.0509329668	0.0000000000
O	1.8275187096	0.7818516966	0.0000000000
N	1.2681390469	1.8617684366	0.0000000000
H	0.2371004680	1.6737740748	0.0000000000

Table S34 Cartesian coordinates for the conformation II of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.8088458458	-1.2899821782	0.0000000000
O	-1.3947492184	-0.2305141240	0.0000000000
H	-1.3559118065	-2.2457193942	0.0000000000
H	0.2905611219	-1.3375086745	0.0000000000
H	0.1934241198	1.5182162391	0.0000000000
N	1.2141830082	1.2796820116	0.0000000000
O	1.8613386208	2.3058261201	0.0000000000

Table S35 Cartesian coordinates for the conformation III of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	-1.3376186125	0.1867697914	0.0000000000
C	-0.7279084184	-0.8625802258	0.0000000000
H	-0.4478783578	-1.3678191040	0.9359197058
H	-0.4478783578	-1.3678191040	-0.9359197058
O	1.5751893483	0.3608771780	0.0000000000
N	1.2207041821	1.5194172083	0.0000000000
H	0.1653902161	1.5311542561	0.0000000000

Table S36 Cartesian coordinates for the conformation IV of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.8234617396	-1.1869343798	0.0000000000
O	1.4925712260	-0.1789230871	0.0000000000
H	0.5045496096	-1.6688056888	0.9372303072
H	0.5045496096	-1.6688056888	-0.9372303072
N	-1.1564855163	1.1299744413	0.0000000000
H	-0.1928433183	1.5521105955	0.0000000000
O	-1.9758033502	2.0213838078	0.0000000000

Table S37 Cartesian coordinates for the conformation V of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.0274744749	1.4619895221	0.0000000000
O	-0.8018497466	2.3891725471	0.0000000000
H	0.3465753665	1.0152942986	0.9347282398
H	0.3465753665	1.0152942986	-0.9347282398
O	0.9677156313	-1.6402955973	0.0000000000
N	-0.2435429197	-1.6238610015	0.0000000000
H	-0.5879992230	-2.6175940675	0.0000000000

Table S38 Cartesian coordinates for the conformation VI of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVQZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	0.9242385535	2.5049649172	0.0000000000
C	0.3059892788	1.4671013856	0.0000000000
H	0.0069321106	0.9668956905	0.9346799534
H	0.0069321106	0.9668956905	-0.9346799534
O	0.5149163985	-1.6714928275	0.0000000000
N	-0.6954213016	-1.6245206357	0.0000000000
H	-1.0635871503	-2.6098442204	0.0000000000

Table S39 Cartesian coordinates for the conformation I of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
H	-1.5357602352	-1.9412091940	0.0000000000
C	-0.8272576634	-1.0970866490	0.0000000000
H	0.2470221401	-1.3334399303	0.0000000000
O	-1.2209156810	0.0525959452	0.0000000000
O	1.8294064255	0.7793377640	0.0000000000
N	1.2700239955	1.8639590088	0.0000000000
H	0.2374810185	1.6758430552	0.0000000000

Table S40 Cartesian coordinates for the conformation II of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.8094032855	-1.2906097548	0.0000000000
O	-1.3996571954	-0.2290513283	0.0000000000
H	-1.3541838263	-2.2486707534	0.0000000000
H	0.2909894818	-1.3356444201	0.0000000000
H	0.1930844774	1.5182738186	0.0000000000
N	1.2149929045	1.2780019289	0.0000000000
O	1.8641774434	2.3077005091	0.0000000000

Table S41 Cartesian coordinates for the conformation III of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	-1.3407872054	0.1883436014	0.0000000000
C	-0.7290843154	-0.8642823867	0.0000000000
H	-0.4480606440	-1.3697448746	0.9365730183
H	-0.4480606440	-1.3697448746	-0.9365730183
O	1.5786181894	0.3603061925	0.0000000000
N	1.2220731151	1.5226321507	0.0000000000
H	0.1653015043	1.5324901914	0.0000000000

Table S42 Cartesian coordinates for the conformation IV of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.8225215541	-1.1868676998	0.0000000000
O	1.4971906547	-0.1779760025	0.0000000000
H	0.5016955066	-1.6681760603	0.9377866584
H	0.5016955066	-1.6681760603	-0.9377866584
N	-1.1533403455	1.1281217934	0.0000000000
H	-0.1899404770	1.5547240048	0.0000000000
O	-1.9798223994	2.0183500246	0.0000000000

Table S43 Cartesian coordinates for the conformation V of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.0264168958	1.4572184062	0.0000000000
O	-0.8083591754	2.3832394821	0.0000000000
H	0.3511740081	1.0126557356	0.9353746690
H	0.3511740081	1.0126557356	-0.9353746690
O	0.9690739585	-1.6354245316	0.0000000000
N	-0.2463878789	-1.6173722128	0.0000000000
H	-0.5902580246	-2.6129726150	0.0000000000

Table S44 Cartesian coordinates for the conformation VI of the $H_2CO\cdots HNO$ dimer as optimized at the CCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	0.9252283866	2.5063101196	0.0000000000
C	0.3056679485	1.4646115700	0.0000000000
H	0.0066080483	0.9636948656	0.9352682877
H	0.0066080483	0.9636948656	-0.9352682877
O	0.5167492690	-1.6668765685	0.0000000000
N	-0.6979158448	-1.6216449491	0.0000000000
H	-1.0629458559	-2.6097899032	0.0000000000

Table S45 Cartesian coordinates for the cation of conformation I of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
H	-1.8016117293	-1.6342223668	0.0000000000
C	-0.8733891731	-1.0665534957	0.0000000000
H	0.1042949784	-1.5502341548	0.0000000000
O	-0.9808471034	0.1761752936	0.0000000000
O	2.3981228969	1.6360616366	0.0000000000
N	1.2566282887	1.7540572429	0.0000000000
H	-0.1031981582	0.6847158442	0.0000000000

Table S46 Cartesian coordinates for the cation of conformation II of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.6995729536	-1.2115250987	0.0000000000
O	-0.9313192973	0.0144766699	0.0000000000
H	-1.5654237247	-1.8705187111	0.0000000000
H	0.3228519349	-1.5921851989	0.0000000000
H	-0.0995362409	0.5975822618	0.0000000000
N	1.3937232490	1.4651943703	0.0000000000
O	1.5792770326	2.5969757068	0.0000000000

Table S47 Cartesian coordinates for the cation of conformation III of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	-0.2607560663	-0.1701286099	0.0000000000
C	-1.0054325788	-1.1443614367	0.0000000000
H	-1.3340835111	-1.5743474924	0.9498183478
H	-1.3340835111	-1.5743474924	-0.9498183478
O	2.3284911070	1.8849138917	0.0000000000
N	1.1871004268	1.8505450904	0.0000000000
H	0.4187641334	0.7277260493	0.0000000000

Table S48 Cartesian coordinates for the cation of conformation IV of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.8584351820	-1.2574566777	0.0000000000
O	0.0904083491	-0.3014662938	0.0000000000
H	1.1967319782	-1.6802589232	0.9496885313
H	1.1967319782	-1.6802589232	-0.9496885313
N	-1.4971839915	1.6114028011	0.0000000000
H	-0.6049103013	0.5839368934	0.0000000000
O	-1.2402131948	2.7241011235	0.0000000000

Table S49 Cartesian coordinates for the cation of conformation V of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.0220744822	0.6851069183	0.0000000000
O	-1.2214688200	1.1330177731	0.0000000000
H	0.5886860568	0.9700275794	0.9024359194
H	0.5886860568	0.9700275794	-0.9024359194
O	0.9661366018	-1.5585267101	0.0000000000
N	0.0014098309	-0.8744816925	0.0000000000
H	-0.9455242085	-1.3251714475	0.0000000000

Table S50 Cartesian coordinates for the cation of conformation IV of the $H_2CO\cdots HNO$ dimer as optimized at the UCCSD(T)/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
O	1.3270454120	1.5633046168	0.0000000000
C	0.2001790935	1.0569598939	0.0000000000
H	-0.3634228115	1.0597282474	0.9479216156
H	-0.3634228115	1.0597282474	-0.9479216156
O	0.4093493803	-0.8755127796	0.0000000000
N	-0.6853766590	-1.4156771553	0.0000000000
H	-0.5243516039	-2.4485310706	0.0000000000

Table S51 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation I at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	61.42
2	101.80
3	101.93
4	132.30
5	181.83
6	262.61
7	1195.73
8	1265.66
9	1524.53
10	1532.54
11	1607.92
12	1751.60
13	2952.05
14	3039.97
15	3068.82

Table S52 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation II at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	72.15
2	112.51
3	117.74
4	129.67
5	177.39
6	1192.66
7	1267.58
8	1528.90
9	1541.67
10	1573.22
11	1754.32
12	2947.08
13	3027.80
14	3051.35

Table S53 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation III at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	116.72
2	125.95
3	196.39
4	285.59
5	294.41
6	444.28
7	1175.31
8	1259.19
9	1525.20
10	1553.28
11	1606.86
12	1743.48
13	2956.63
14	2974.33
15	3031.74

Table S54 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation IV at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	107.93
2	157.73
3	219.63
4	1183.85
5	1262.06
6	1529.64
7	1537.40
8	1582.22
9	1759.45
10	2945.28
11	2995.80
12	3018.66

Table S55 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation V at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	76.84
2	117.51
3	184.03
4	203.81
5	1181.05
6	1255.75
7	1523.27
8	1531.40
9	1585.87
10	1764.32
11	2940.59
12	2982.64
13	3012.73

Table S56 Harmonic vibrational frequencies (in cm^{-1}) determined for the (neutral) conformation VI at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	58.10
2	86.47
3	105.22
4	158.40
5	192.06
6	1180.99
7	1255.99
8	1521.64
9	1532.57
10	1586.98
11	1763.80
12	2940.69
13	2980.57
14	3014.92

Table S57 Harmonic vibrational frequencies (in cm^{-1}) determined for the (cation) conformation I-IV at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	55.33
2	85.58
3	144.81
4	280.95
5	288.05
6	1125.16
7	1186.54
8	1233.84
9	1462.32
10	1488.51
11	1669.84
12	1944.00
13	2935.55
14	3093.87
15	3236.97

Table S58 Harmonic vibrational frequencies (in cm^{-1}) determined for the (cation) conformation V at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	44.04
2	311.24
3	456.18
4	669.09
5	821.20
6	924.97
7	1173.83
8	1190.47
9	1331.58
10	1342.04
11	1478.89
12	1709.83
13	2956.99
14	3015.93
15	3161.09

Table S59 Harmonic vibrational frequencies (in cm^{-1}) determined for the (cation) conformation VI at the CCSD(T)AVTZ level of theory.

Vibrational number	Frequencies
1	58.01[a]
2	148.71
3	238.97
4	392.90
5	638.16
6	767.76
7	885.35
8	1109.11
9	1300.64
10	1466.25
11	1493.18
12	1555.16
13	2888.84
14	3005.00
15	3169.63

[a] Imaginary, but reoptimizing along this normal mode did not eliminate.