Raw data used for determining the ionization energies of dimers of small molecular clusters

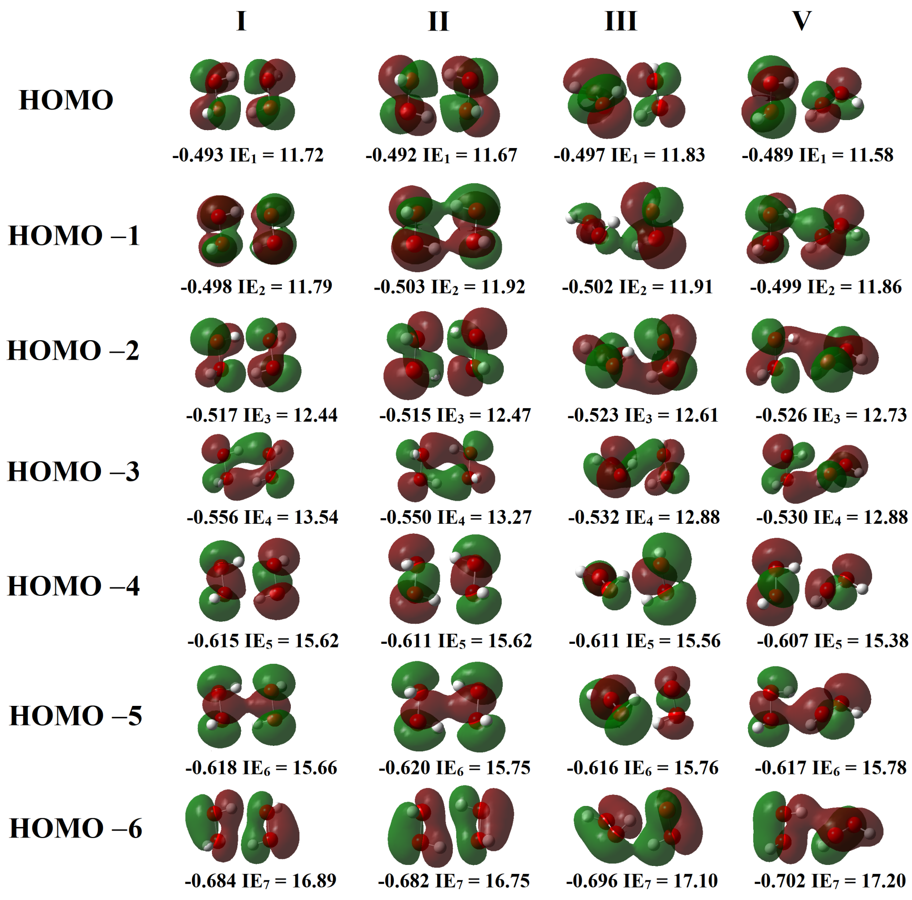

Figure 1: Molecular orbital plots generated at HF/aug-cc-pVTZ for the conformations of the H_2O_2 dimer. The orbital energies are given in hartrees while the corresponding composite IEs are provided in eV.

Table 1: Vertical ionization energies (IEs) for the conformation I of the H_2O_2 dimer as determined 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.

IE	$\mathbf{E}_{\text{AVDZ}}$	$\mathbf{E}_{\text{AVTZ}}$	$\mathbf{E}_{\text{AVQZ}}$	$\mathbf{E}_{\text{CBS[DT]}}$	$\mathbf{E}_{\text{CBS[TQ]}}$
1	11.31	11.54	11.63	11.62	11.69
2	11.37	11.61	11.70	11.70	11.76
3	12.05	12.27	12.36	12.35	12.41
4	13.16	13.37	13.46	13.45	13.51
5	15.32	15.48	15.56	15.53	15.60
6	15.34	15.51	15.59	15.57	15.63
7	16.58	16.74	16.82	16.80	16.87
8	18.05	18.19	18.26	18.24	18.31
9	18.54	18.64	18.71	18.67	18.75
10	18.64	18.74	18.81	18.78	18.85

Table 2: Core correlation effects for the vertical ionization energies (IEs) for the conformation I of the H_2O_2 dimer as determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IE	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	Δ_{CV}**(DZ)**	Δ_{CV}**(TZ)**
1	11.32	11.56	0.008	0.03
2	11.38	11.63	0.008	0.03
3	12.06	12.29	0.008	0.03
4	13.17	13.38	0.008	0.03
5	15.33	15.49	0.01	0.02
6	15.35	15.52	0.01	0.03
7	16.60	16.75	0.01	0.02
8	18.06	18.20	0.01	0.02
9	18.55	18.64	0.01	0.02
10	18.65	18.75	0.01	0.02

Table 3: Raw values used for computing the vertical ionization energies (IEs) for the conformation I of the H_2O_2 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
Ground	-302.47404008086778	-302.72151791662054	-302.79771503118968
1	-302.05841524219119	-302.29733224620679	-302.37015656031366
2	-302.05606290647114	-302.29480205835358	-302.36763371700397
3	-302.03110849075875	-302.27050513077216	-302.34340387687075
4	-301.99027906784283	-302.23011419395255	-302.30319275451569
5	-301.91108551055800	-302.15274347738722	-302.22602341749064
6	-301.91028387017531	-302.15164546378423	-302.22487115378965
7	-301.86466234487330	-302.10632311655110	-302.17959147261763
8	-301.81078028031720	-302.05307334030812	-302.12657759896200
9	-301.79266447816065	-302.03661186734570	-302.11024764915339
10	-301.78895136595548	-302.03271480162562	-302.10635329399366

Table 4: Raw values used for computing the vertical ionization energies (IEs) for the conformation I of the H_2O_2 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	-302.63804053463946	-302.94713544259230
1	-302.22175269674989	-302.52119441909537
2	-302.21939875034911	-302.51866529864412
3	-302.19444006723148	-302.49445075323973
4	-302.15364025361453	-302.45418774973064
5	-302.07442277801289	-302.37701196294273
6	-302.07360630668597	-302.37588187905538
7	-302.02794611644100	-302.33065167697214
8	-301.97410622257871	-302.27754707230395
9	-301.95617508209722	-302.26117613615685
10	-301.95244859277159	-302.25725839560215

Table 5: Raw values used for computing the vertical ionization energies (IEs) for the conformation I of the H_2O_2 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	-302.48552675666889	-302.73320751466423
1	-302.06954487544289	-302.30849887368726
2	-302.06719026596232	-302.30595513988669
3	-302.04222199749853	-302.28168963630526
4	-302.00141506555798	-302.24134018151915
5	-301.92214817790625	-302.16399114164909
6	-301.92134406902471	-302.16288265773164
7	-301.87567765680927	-302.11758700672789
8	-301.82182393270364	-302.06439108204927
9	-301.80388838683876	-302.04806298073692
10	-301.80017475190203	-302.04415162805776

Table 6: Cartesian coordinates of the conformation I of the H_2O_2 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	1.4699449294	0.7535129510	0.0143346538
O	1.3567781200	-0.7025695461	0.1139808231
O	-1.3588137486	0.7016535604	-0.1161263356
O	-1.4714028534	-0.7541269046	-0.0101337673
H	1.7934521680	-0.9629203001	-0.7085773199
H	0.5283701706	0.9756140302	-0.1093572143
H	-1.7893383286	0.9650818076	0.7087114945
H	-0.5289904574	-0.9762455983	0.1071676657

Table 7: Cartesian coordinates of the cation of conformation I of the H_2O_2 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	1.5987248426	0.5399307034	0.2968528134
O	0.9287143627	-0.4053180257	-0.5857365969
O	-1.8384171063	0.5413772542	0.1695453294
O	-1.2471108146	-0.6013675767	0.4649601731
H	1.4830257329	-1.2064325944	-0.5119657702
H	1.9259912732	1.1836566506	-0.3580137231
H	-2.7217717429	0.4736081464	0.5987514777
H	-0.1291565475	-0.5254545579	-0.0743937035

Table 8: Vertical ionization energies (IEs) for the conformation II of the H_2O_2 dimer as determined 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.

IE	$\mathbf{E}_{\text{AVDZ}}$	$\mathbf{E}_{\text{AVTZ}}$	$\mathbf{E}_{\text{AVQZ}}$	$\mathbf{E}_{\text{CBS[DT]}}$	$\mathbf{E}_{\text{CBS[TQ]}}$
1	11.26	11.50	11.59	11.58	11.64
2	11.52	11.75	11.84	11.83	11.89
3	12.09	12.30	12.39	12.38	12.44
4	12.88	13.10	13.19	13.18	13.24
5	15.32	15.47	15.55	15.53	15.60
6	15.43	15.60	15.68	15.66	15.72
7	16.44	16.60	16.68	16.66	16.73
8	18.12	18.26	18.34	18.31	18.38
9	18.60	18.70	18.77	18.74	18.81
10	18.62	18.72	18.79	18.75	18.83

Table 9: Core correlation effects for the vertical ionization energies (IEs) for the conformation II of the H_2O_2 dimer as determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IE	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVDZ}}$	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVTZ}}$	Δ_{CV}**(DZ)**	Δ_{CV}**(TZ)**
1	11.27	11.51	0.008	0.03
2	11.53	11.77	0.008	0.03
3	12.10	12.32	0.008	0.03
4	12.89	13.11	0.008	0.03
5	15.33	15.48	0.01	0.02
6	15.44	15.61	0.01	0.03
7	16.45	16.61	0.01	0.02
8	18.14	18.28	0.01	0.02
9	18.61	18.71	0.01	0.02
10	18.63	18.72	0.01	0.02

Table 10: Raw values used for computing the vertical ionization energies (IEs) for the conformation II of the H_2O_2 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
Ground	-302.47365389143391	-302.72126297596384	-302.79751227420905
1	-302.05978737469650	-302.29871784395260	-302.37157999335875
2	-302.05043637091580	-302.28942374335668	-302.36234774251972
3	-302.02932388731546	-302.26911017996667	-302.34210860547063
4	-302.00019779498541	-302.23986247225400	-302.31291928168287
5	-301.91074199461502	-302.15266517428472	-302.22602050902537
6	-301.90657336184654	-302.14810117078059	-302.22140140048441
7	-301.86946301393999	-302.11115799736331	-302.18445176576006
8	-301.80766718211373	-302.05005598470098	-302.12361851571785
9	-301.79010887358055	-302.03404258360331	-302.10773542872062
10	-301.78921654999260	-302.03338535885865	-302.10708898116366

Table 11: Raw values used for computing the vertical ionization energies (IEs) for the conformation II of the H_2O_2 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	-302.63764133814931	-302.94689827260061
1	-302.22310944434508	-302.52258858003910
2	-302.21376986282525	-302.51333684237187
3	-302.19265103099963	-302.49310737479607
4	-302.16353660394793	-302.46390014107106
5	-302.07406692277141	-302.37696752875098
6	-302.06989350804821	-302.37237118997018
7	-302.03272720508238	-302.33548731713222
8	-301.97097348863849	-302.27455003930521
9	-301.95359849417758	-302.25860810314509
10	-301.95272030491833	-302.25797622716698

Table 12: Raw values used for computing the vertical ionization energies (IEs) for the conformation II of the H_2O_2 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	-302.48513670087738	-302.73296572855725
1	-302.07091090354851	-302.30988893570731
2	-302.06156615064629	-302.30059897939179
3	-302.04043337138614	-302.28031793276733
4	-302.01132922844255	-302.25108517854841
5	-301.92179348998741	-302.16392530332939
6	-301.91764027358084	-302.15936013974488
7	-301.88047129739442	-302.12242931393672
8	-301.81870099540441	-302.06138253521493
9	-301.80133168629516	-302.04549559665634
10	-301.80044172762422	-302.04485390436173

Table 13: Cartesian coordinates of the conformation II of the H_2O_2 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	1.4662315045	0.7135640696	-0.4003652869
O	1.3409792674	-0.7074718640	-0.0795368272
O	-1.3387051998	0.7072732028	-0.0782387294
O	-1.4647141838	-0.7133123932	-0.4012551605
H	1.7792343246	-0.7318453844	0.7815445128
H	0.5341419803	0.9814835463	-0.2991138543
H	-0.5325470378	-0.9816757937	-0.3018812134
H	-1.7846206553	0.7319846166	0.7788465588

Table 14: Cartesian coordinates of the cation of conformation II of the H_2O_2 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	1.5521844730	0.7168264266	0.2084115324
O	0.9884427242	-0.4927640611	-0.3748614002
O	-1.8829732789	0.4127779932	-0.1326894464
O	-1.2409501514	-0.4972992606	0.5761134866
H	1.5720460897	-1.1962492093	-0.0298440728
H	1.8935906660	1.1515089611	-0.5946249316
H	-0.0943083989	-0.5201492898	0.0931517296
H	-2.7880321237	0.4253484399	0.2543431024

Table 15: Vertical ionization energies (IEs) for the conformation III of the H_2O_2 dimer as determined 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.

IE	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
1	11.42	11.65	11.74	11.73	11.80
2	11.51	11.74	11.83	11.82	11.88
3	12.23	12.44	12.53	12.52	12.58
4	12.49	12.71	12.79	12.78	12.85
5	15.25	15.42	15.50	15.47	15.54
6	15.46	15.62	15.70	15.67	15.74
7	16.79	16.95	17.03	17.01	17.08
8	17.75	17.90	17.98	17.96	18.02
9	18.52	18.61	18.68	18.64	18.72
10	18.64	18.73	18.80	18.76	18.84

Table 16: Core correlation effects for the vertical ionization energies (IEs) for the conformation III of the H_2O_2 dimer as determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IE	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVDZ}}$	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVTZ}}$	Δ_{CV}**(DZ)**	Δ_{CV}**(TZ)**
1	11.43	11.67	0.008	0.03
2	11.51	11.75	0.008	0.03
3	12.24	12.46	0.008	0.03
4	12.50	12.72	0.008	0.03
5	15.27	15.43	0.01	0.02
6	15.48	15.63	0.01	0.02
7	16.80	16.96	0.01	0.02
8	17.76	17.92	0.01	0.02
9	18.52	18.62	0.01	0.02
10	18.64	18.74	0.01	0.02

Table 17: Raw values used for computing the vertical ionization energies (IEs) for the conformation III of the H_2O_2 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
Ground	-302.47152500047196	-302.71870126228447	-302.79499630731016
1	-302.05195170347525	-302.29053514160557	-302.36346180601106
2	-302.04872719483774	-302.28733163561770	-302.36030257489256
3	-302.02224139474015	-302.26146270024179	-302.33453401332895
4	-302.01243726119071	-302.25175153301262	-302.32480455353215
5	-301.91093817286122	-302.15221471173669	-302.22555609724242
6	-301.90321478531320	-302.14469798642642	-302.21808781636253
7	-301.85450561406526	-302.09571792381297	-302.16914175756779
8	-301.81920404897539	-302.06073359424522	-302.13427405757415
9	-301.79102703844006	-302.03478150483102	-302.10852060413754
10	-301.78662435094293	-302.03037652217813	-302.10412849995919

Table 18: Raw values used for computing the vertical ionization energies (IEs) for the conformation III of the H_2O_2 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	-302.63546396259960	-302.94433384141962
1	-302.21523327118655	-302.51442430685751
2	-302.21202253296417	-302.51125074602896
3	-302.18553524985896	-302.48546865010326
4	-302.17572552848901	-302.47576150236875
5	-302.07421104097369	-302.37648661350215
6	-302.06650857130779	-302.36900035148705
7	-302.01773772107197	-302.32008673758185
8	-301.98243224869213	-302.28517519568391
9	-301.95449656492798	-302.25936685566268
10	-301.95008860567248	-302.25496980549616

Table 19: Raw values used for computing the vertical ionization energies (IEs) for the conformation III of the H_2O_2 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	-302.48301771826010	-302.73043763145205
1	-302.06309064808607	-302.30174987467666
2	-302.05987431963888	-302.29854015993646
3	-302.03337918983738	-302.27270792977959
4	-302.02356725669779	-302.26299264886768
5	-301.92200591173156	-302.16350016695526
6	-301.91429999893245	-302.15600449816543
7	-301.86553601525577	-302.10702753282555
8	-301.83022422973124	-302.07205668402850
9	-301.80227686185276	-302.04628767109335
10	-301.79786824348139	-302.04188178799325

Table 20: Cartesian coordinates of the conformation III of the H_2O_2 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	-1.5002722405	0.1078974676	-0.5674586875
O	-1.0570708835	-0.5079019003	0.6844094267
O	1.6494195142	-0.7299054845	-0.3410684346
O	1.4657891989	0.5605230353	0.3178358449
H	-0.3523127855	0.1204439466	0.9257218463
H	-2.3848413206	0.3965600778	-0.3063962073
H	1.4295558755	1.1431522174	-0.4537898177
H	0.7497326414	-1.0907693600	-0.2592539708

Table 21: Cartesian coordinates of the cation of conformation III of the H_2O_2 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	-1.9228081755	-0.1001022707	-0.1951899355
O	-1.1638725240	0.6544947671	0.5779345911
O	1.4170670512	-0.9621654132	0.2025092712
O	1.0638283381	0.3475950526	-0.3275917367
H	-0.0129764166	0.5198934529	0.1178252017
H	-2.8285979673	0.0112714485	0.1737952275
H	1.7387353610	0.9340267716	0.0663301375
H	1.7086243332	-1.4050138088	-0.6156127567

Table 22: Vertical ionization energies (IEs) for the conformation V of the H_2O_2 dimer as determined 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.

IE	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
1	11.18	11.41	11.50	11.49	11.55
2	11.45	11.69	11.78	11.77	11.83
3	12.35	12.56	12.65	12.63	12.70
4	12.50	12.71	12.80	12.79	12.85
5	15.06	15.22	15.30	15.28	15.35
6	15.48	15.64	15.72	15.69	15.76
7	16.90	17.06	17.13	17.11	17.18
8	17.65	17.81	17.88	17.86	17.92
9	18.35	18.43	18.50	18.46	18.54
10	18.65	18.75	18.81	18.78	18.85

Table 23: Core correlation effects for the vertical ionization energies (IEs) for the conformation V of the H_2O_2 dimer as determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IE	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVDZ}}$	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVTZ}}$	Δ_{CV}**(DZ)**	Δ_{CV}**(TZ)**
1	11.18	11.42	0.008	0.03
2	11.46	11.70	0.008	0.03
3	12.36	12.57	0.008	0.03
4	12.51	12.73	0.008	0.03
5	15.07	15.24	0.01	0.03
6	15.49	15.65	0.01	0.02
7	16.91	17.07	0.01	0.02
8	17.66	17.82	0.01	0.02
9	18.35	18.44	0.01	0.02
10	18.66	18.75	0.01	0.02

Table 24: Raw values used for computing the vertical ionization energies (IEs) for the conformation V of the H_2O_2 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
Ground	-302.47050554005915	-302.71800654470354	-302.79435925469670
1	-302.05983067447022	-302.29872460148630	-302.37171941263119
2	-302.04962761010921	-302.28856720091733	-302.36158410631731
3	-302.01676668424841	-302.25647389825218	-302.32963068362818
4	-302.01098233214617	-302.25077783455885	-302.32395485499029
5	-301.91702417456401	-302.15858117265805	-302.23196717500434
6	-301.90154789457944	-302.14338148616667	-302.21684537982446
7	-301.84956565985226	-302.09116291805861	-302.16467820838568
8	-301.82187327446422	-302.06366979370273	-302.13728745108716
9	-301.79629085747547	-302.04065883851393	-302.11447126167457
10	-301.78497533237191	-302.02915112442213	-302.10299688585133

Table 25: Raw values used for computing the vertical ionization energies (IEs) for the conformation V of the H_2O_2 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	-302.63441084213508	-302.94366408593584
1	-302.22308036106097	-302.52263303211816
2	-302.21288412552275	-302.51249635739265
3	-302.18001764182748	-302.48051732663896
4	-302.17424751114464	-302.47484274519479
5	-302.08026013378242	-302.38286034401699
6	-302.06480045726795	-302.36771115319914
7	-302.01275719269432	-302.31556520437641
8	-301.98506071245339	-302.28813311065949
9	-301.95972902867868	-302.26528368713400
10	-301.94841179913237	-302.25377821152392

Table 26: Raw values used for computing the vertical ionization energies (IEs) for the conformation V of the H_2O_2 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	-302.48198599564341	-302.72976513296965
1	-302.07095738732852	-302.30994964326260
2	-302.06076065126365	-302.29980121430509
3	-302.02787816607872	-302.26773670887491
4	-302.02210516578066	-302.26204723352089
5	-301.92808185643219	-302.16988769658752
6	-301.91261379998599	-302.15470771045625
7	-301.86057777410991	-302.10249441375441
8	-301.83287301746395	-302.07500504335775
9	-301.80752401904533	-302.05218985243755
10	-301.79620851675622	-302.04068263715868

Table 27: Cartesian coordinates of the conformation V of the H_2O_2 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	1.9305662881	0.3711746603	-0.4802760376
O	1.0074752020	-0.1583987755	0.5192123701
O	-1.5852191183	0.9188031698	0.0049163471
O	-1.6043979518	-0.4896840245	-0.3892527536
H	0.4259577730	-0.7013365200	-0.0395302037
H	2.7420042638	-0.0813674263	-0.2134750559
H	-2.2407031319	-0.8345585416	0.2514875865
H	-0.6756833249	0.9753674578	0.3469177471

Table 28: Cartesian coordinates of the cation of conformation V of the H_2O_2 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	1.4659238624	0.0938554948	-0.7822871497
O	1.0515618231	-0.1057009522	0.5991175091
O	-1.2994660468	0.4640120846	0.4962492739
O	-1.8214412873	-0.2715125033	-0.4686444048
H	1.2759466773	-1.0417230262	0.7638600031
H	2.1930866787	0.7302327331	-0.6526269410
H	-2.7611326951	0.0184335408	-0.5114415258
H	-0.1044790123	0.1124026285	0.5557732352

Table 29: Cartesian coordinates of the conformation IV of the H_2O_2 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	-1.4657245878	0.5605462507	0.3178316621
O	-1.6493839791	-0.7299187751	-0.3409863473
O	1.0571171482	-0.5078900133	0.6844844283
O	1.5001431852	0.1077062121	-0.5675563614
H	-0.7496845341	-1.0907377192	-0.2590964349
H	-1.4294059708	1.1430978680	-0.4538523816
H	2.3846094947	0.3967431639	-0.3065524428
H	0.3523292437	0.1204530130	0.9257278777

Table 30: Cartesian coordinates of the conformation VI of the H_2O_2 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	1.6043971631	-0.4896835960	-0.3892534626
O	1.5852179937	0.9188034407	0.0049162319
O	-1.0074755477	-0.1583998782	0.5192137094
O	-1.9305647704	0.3711751810	-0.4802755933
H	0.6756824992	0.9753670486	0.3469185418
H	2.2407033401	-0.8345580165	0.2514859442
H	-2.7420033088	-0.0813671313	-0.2134766953
H	-0.4259573692	-0.7013370484	-0.0395286761

Table 31: Vertical ionization energies (IEs) for the conformation I of the H_2O_2 dimer as determined 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.

IE	$\mathbf{E}_{\text{AVDZ}}$	$\mathbf{E}_{\text{AVTZ}}$	$\mathbf{E}_{\text{AVQZ}}$	$\mathbf{E}_{\text{CBS[DT]}}$	$\mathbf{E}_{\text{CBS[TQ]}}$
1	11.31	11.54	11.63	11.62	11.68
2	12.37	12.58	12.66	12.65	12.71
3	15.23	15.38	15.46	15.44	15.51
4	17.25	17.40	17.48	17.46	17.52
5	18.47	18.55	18.62	18.58	18.65
6	20.65	21.37	21.56	21.62	21.68
7	22.30	23.02	23.22	23.27	23.33
8	23.13	23.78	23.96	24.01	24.07
9	23.64	24.28	24.46	24.51	24.57
10	25.68	26.32	26.50	26.54	26.61

Table 32: Core correlation effects for the vertical ionization energies (IEs) of the H_2O_2 molecule as determined using EOMIP-CCSD/aug-cc-pCVnZ (n = D and T) approaches. The values are given in eV.

IE	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	$\Delta_{\text{CV}}\mathbf{(DZ)}$	$\Delta_{\text{CV}}\mathbf{(TZ)}$
1	11.32	11.55	0.008	0.03
2	12.38	12.59	0.007	0.03
3	15.24	15.40	0.006	0.02
4	17.26	17.41	0.006	0.02
5	18.48	18.55	0.01	0.02
6	20.68	21.40	0.07	0.15
7	22.32	23.06	0.07	0.15
8	23.16	23.82	0.07	0.15
9	23.67	24.31	0.07	0.14
10	25.71	26.35	0.07	0.14

Table 33: Raw values used for computing the vertical ionization energies (IEs) of the H_2O_2 molecule as determined using the frozen-core EOMIP-CCSD/aug-cc-pVnZ (n = D, T, and Q) approaches. The values are given in hartrees.

State	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
Ground	-151.22990065454110	-151.35396532913879	-151.39234773807414
1	-150.81427626603733	-150.92998110274183	-150.96509367937642
2	-150.77525446746421	-150.89181263130180	-150.92707779808958
3	-150.67010992906970	-150.78860808153848	-150.82413584425242
4	-150.59593700740768	-150.71446686021557	-150.75015076997138
5	-150.55106128178292	-150.67232466334264	-150.70826357540523
6	-150.47100614774018	-150.56872790359060	-150.59991668650173
7	-150.41050568381709	-150.50800156036522	-150.53906537743592
8	-150.37978990261621	-150.48008274793415	-150.51172310906190
9	-150.36131313523722	-150.46175012009999	-150.49345427003499
10	-150.28628417172590	-150.38684511722749	-150.41842681291379

Table 34: Raw values used for computing the vertical ionization energies (IEs) of the H_2O_2 molecule 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	-151.31174332874266	-151.46685486938182
1	-150.89548707751828	-151.04115782124774
2	-150.85646627420334	-151.00311964130785
3	-150.75130171950858	-150.90016318892401
4	-150.67706180890505	-150.82615825132024
5	-150.63245170417144	-150.78421065677850
6	-150.54928181877105	-150.67472710653055
7	-150.48887562670851	-150.61405682843076
8	-150.45796331356863	-150.58628250299265
9	-150.43954063175434	-150.56809219672471
10	-150.36461499819089	-150.49330011197961

Table 35: Raw values used for computing the vertical ionization energies (IEs) of the H_2O_2 molecule 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	-151.23561514802498	-151.35994489505543
1	-150.81964736768444	-150.93542709029472
2	-150.78060898743624	-150.89729398356133
3	-150.67540668445218	-150.79414159149388
4	-150.60116132858252	-150.72001119081645
5	-150.55653302569664	-150.67808655544260
6	-150.47570433450588	-150.57335160438481
7	-150.41525668353646	-150.51263896649149
8	-150.38437894274313	-150.48473405952288
9	-150.36591234849251	-150.46643251168007
10	-150.29093538432255	-150.39156430582261

Table 36: Cartesian coordinates of the H_2O_2 molecule 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	-0.7220653092	0.1100444099	-0.2657911363
O	0.7221279340	-0.1102225953	-0.2655383223
H	-1.0047137280	-0.6459976584	0.2657586513
H	1.0046511032	0.6461758438	0.2655708074

Table 37: 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	$\mathbf{E}_{\text{AVDZ}}$	$\mathbf{E}_{\text{AVTZ}}$	$\mathbf{E}_{\text{AVQZ}}$	$\mathbf{E}_{\text{CBS[DT]}}$	$\mathbf{E}_{\text{CBS[TQ]}}$
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 38: 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	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	$\Delta_{\text{CV}}\mathbf{(DZ)}$	$\Delta_{\text{CV}}\mathbf{(TZ)}$
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 39: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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

Table 40: 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 #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
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 41: 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 #	$\mathbf{E}^{FC}_{ACVDZ}$	$\mathbf{E}^{FC}_{ACVTZ}$
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 42: 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	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
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 43: 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	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	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 44: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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 45: 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 #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
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 46: 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 #	$\mathbf{E}_{ACVDZ}^{FC}$	$\mathbf{E}_{ACVTZ}^{FC}$
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 47: 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	$\mathbf{E}_{\text{AVDZ}}$	$\mathbf{E}_{\text{AVTZ}}$	$\mathbf{E}_{\text{AVQZ}}$	$\mathbf{E}_{\text{CBS[DT]}}$	$\mathbf{E}_{\text{CBS[TQ]}}$
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 48: 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	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	$\Delta_{\text{CV}}\mathbf{(DZ)}$	$\Delta_{\text{CV}}\mathbf{(TZ)}$
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 49: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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 50: 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 51: 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 52: 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	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
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 53: 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	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVDZ}}$	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVTZ}}$	$\Delta_{\mathrm{CV}}\mathbf{(DZ)}$	$\Delta_{\mathrm{CV}}\mathbf{(TZ)}$
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 54: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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 55: 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 #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
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 56: 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 #	$\mathbf{E}_{ACVDZ}^{FC}$	$\mathbf{E}_{ACVTZ}^{FC}$
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 57: 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	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
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 58: 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	$\mathbf{E}^{\text{FC}}_{\text{ACVDZ}}$	$\mathbf{E}^{\text{FC}}_{\text{ACVTZ}}$	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 59: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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 60: 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 #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
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 61: 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 #	$\mathbf{E}^{FC}_{ACVDZ}$	$\mathbf{E}^{FC}_{ACVTZ}$
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 62: 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	$\mathbf{E}_{\mathrm{AVDZ}}$	$\mathbf{E}_{\mathrm{AVTZ}}$	$\mathbf{E}_{\mathrm{AVQZ}}$	$\mathbf{E}_{\mathrm{CBS[DT]}}$	$\mathbf{E}_{\mathrm{CBS[TQ]}}$
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 63: 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	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVDZ}}$	$\mathbf{E}^{\mathrm{FC}}_{\mathrm{ACVTZ}}$	$\Delta_{\mathrm{CV}}\mathbf{(DZ)}$	$\Delta_{\mathrm{CV}}\mathbf{(TZ)}$
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 64: 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	$\mathbf{E}_{AVDZ}$	$\mathbf{E}_{AVTZ}$	$\mathbf{E}_{AVQZ}$
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 65: 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 #	$\mathbf{E}_{ACVDZ}$	$\mathbf{E}_{ACVTZ}$
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 66: 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 #	$\mathbf{E}^{FC}_{ACVDZ}$	$\mathbf{E}^{FC}_{ACVTZ}$
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 67: 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 68: 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 69: 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 70: 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 71: 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 72: 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 73: 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 74: 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