Eletronic Supplementary Information

Probing the geometry reorganization from solution to gas-phase in putrescine derivatives by IRMPD, ^{1}H-NMR and theoretical calculations

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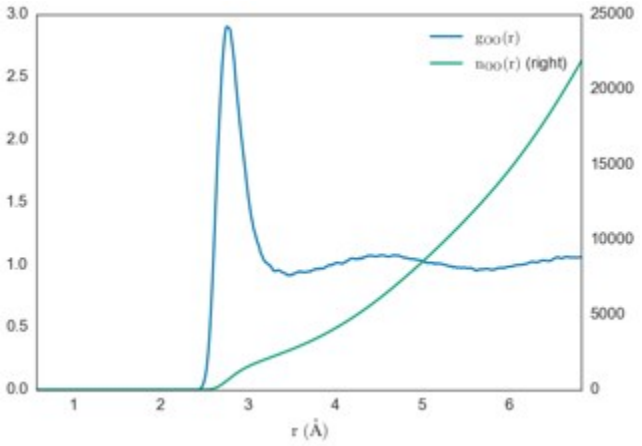

Figure S1. Oxygen-oxygen radial distribution function

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(E)-H2Et2-2H+.log
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.312809	-0.257750	0.370677
2	6	0	-0.488885	-1.191003	-0.159469
3	1	0	-0.055356	0.729164	0.653445
4	1	0	-0.071476	-2.167806	-0.404486
5	6	0	1.750352	-0.551397	0.719502
6	1	0	2.004524	-1.595750	0.526903
7	1	0	1.952887	-0.337254	1.773115
8	6	0	-1.962055	-1.135992	-0.464549
9	1	0	-2.460881	-1.993309	-0.001063
10	1	0	-2.132587	-1.212425	-1.544035
11	7	0	2.746116	0.284688	-0.072603
12	1	0	2.566665	1.283848	0.079336
13	7	0	-2.694404	0.093105	0.010645
14	1	0	-2.553356	0.213732	1.020468
15	6	0	4.217705	0.009495	0.261567
16	6	0	5.135550	0.892810	-0.568268
17	1	0	4.375245	-1.053955	0.067136
18	1	0	4.320869	0.192409	1.333747
19	1	0	6.170700	0.662051	-0.301199
20	1	0	5.028709	0.707167	-1.641902
21	1	0	4.978550	1.957293	-0.365969
22	6	0	-4.208149	0.068442	-0.260019
23	6	0	-4.866427	1.344829	0.236780
24	1	0	-4.586799	-0.821269	0.248258
25	1	0	-4.316178	-0.065360	-1.338817
26	1	0	-5.938059	1.282847	0.026913
27	1	0	-4.756240	1.473922	1.318409
28	1	0	-4.487813	2.234107	-0.277636
29	1	0	-2.309142	0.933240	-0.434512
30	1	0	2.604799	0.126954	-1.077064

:::::::::::::::
(E)-H2Et2-H+.log
:::::::::::::::

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.547437	-1.391203	-0.208778
2	6	0	-0.208179	-0.524281	0.480959
3	1	0	0.108593	-2.322820	-0.570672
4	1	0	0.245713	0.391580	0.855714
5	6	0	2.004415	-1.201690	-0.524897
6	1	0	2.094342	-1.094995	-1.616264

7	1	0	2.534219	-2.144170	-0.287572
8	6	0	-1.652427	-0.760167	0.781306
9	1	0	-1.985472	-1.761254	0.497582
10	1	0	-1.906871	-0.584671	1.830888
11	7	0	2.583751	-0.024112	0.101270
12	1	0	2.687979	-0.188841	1.101515
13	7	0	-2.527116	0.219609	-0.014964
14	1	0	-2.214944	1.174102	0.195493
15	6	0	3.893162	0.359577	-0.453105
16	6	0	4.479670	1.545955	0.305288
17	1	0	3.739472	0.628425	-1.505231
18	1	0	4.607294	-0.482178	-0.438678
19	1	0	5.439812	1.839586	-0.128895
20	1	0	3.804839	2.406669	0.266379
21	1	0	4.658271	1.296737	1.358094
22	6	0	-4.020964	0.117712	0.221319
23	6	0	-4.783825	1.140067	-0.609197
24	1	0	-4.171441	0.264559	1.293429
25	1	0	-4.301162	-0.908089	-0.029545
26	1	0	-5.853134	1.032164	-0.408994
27	1	0	-4.504023	2.166783	-0.351497
28	1	0	-4.634070	0.988958	-1.683118
29	1	0	-2.322472	0.085319	-1.011400

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(E)-Me4-2H+.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.437541	-0.210850	-1.458615
2	1	0	-0.437694	0.211304	1.459038
3	6	0	0.522394	-0.194867	-0.370867
4	6	0	-0.522549	0.195315	0.371290
5	6	0	1.811212	-0.712693	0.210840
6	1	0	1.945605	-1.766290	-0.055482
7	1	0	1.838715	-0.625537	1.299618
8	6	0	-1.811374	0.713131	-0.210406
9	1	0	-1.945834	1.766694	0.056015
10	1	0	-1.838836	0.626078	-1.299193
11	7	0	3.050494	0.007107	-0.313504
12	7	0	-3.050631	-0.006795	0.313828
13	1	0	3.010033	-0.018403	-1.338488
14	1	0	-3.010260	0.018709	1.338815
15	6	0	4.314144	-0.723657	0.088147
16	1	0	5.169323	-0.196521	-0.335384
17	1	0	4.380231	-0.730084	1.176792
18	1	0	4.273649	-1.742953	-0.297079
19	6	0	3.104901	1.459348	0.093620
20	1	0	3.976000	1.919087	-0.374009
21	1	0	2.195341	1.959765	-0.236778

22	1	0	3.195452	1.509950	1.179620
23	6	0	-4.314326	0.723829	-0.087940
24	1	0	-4.274006	1.743114	0.297334
25	1	0	-4.380287	0.730294	-1.176592
26	1	0	-5.169490	0.196570	0.335468
27	6	0	-3.104844	-1.459044	-0.093298
28	1	0	-3.975923	-1.918878	0.374274
29	1	0	-3.195315	-1.509655	-1.179304
30	1	0	-2.195248	-1.959352	0.237167

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(E)-Me4-H+.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.264989	0.399223	-0.187933
2	6	0	0.533321	-0.144049	-1.116694
3	1	0	0.155441	0.628527	0.790958
4	1	0	0.139330	-0.355194	-2.112508
5	6	0	-1.684998	0.782392	-0.443747
6	6	0	1.981423	-0.504349	-0.907893
7	1	0	-1.877347	1.831420	-0.197447
8	1	0	-1.996306	0.600386	-1.475786
9	1	0	2.558914	-0.160089	-1.788659
10	1	0	2.046636	-1.601165	-0.935685
11	7	0	-2.665661	-0.015285	0.441316
12	7	0	2.537739	-0.025018	0.350258
13	6	0	-4.042981	0.586009	0.431534
14	1	0	-3.982465	1.620057	0.772256
15	1	0	-4.689521	0.010012	1.094441
16	1	0	-4.428975	0.550865	-0.588125
17	6	0	-2.694449	-1.477108	0.090730
18	1	0	-3.114632	-1.581643	-0.910675
19	1	0	-1.675893	-1.861982	0.113324
20	1	0	-3.318057	-2.001634	0.815389
21	6	0	2.984010	1.368121	0.254328
22	1	0	2.167764	2.006942	-0.094444
23	1	0	3.293836	1.721769	1.241519
24	1	0	3.835049	1.490452	-0.439537
25	6	0	3.614262	-0.886846	0.846800
26	1	0	3.950072	-0.519123	1.820148
27	1	0	4.488573	-0.915973	0.172359
28	1	0	3.244750	-1.907700	0.980748
29	1	0	-2.303900	0.055865	1.398021

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PES_(E)-Me4-H+.log

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Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.152599	2.237536	-0.706969
2	6	0	-0.758999	1.783498	0.143805
3	1	0	0.456753	3.278445	-0.671189
4	1	0	-1.046756	0.736927	0.101493
5	6	0	0.816679	1.357227	-1.714346
6	6	0	-1.433744	2.650520	1.160048
7	1	0	1.901207	1.467699	-1.701314
8	1	0	0.558960	0.312989	-1.551067
9	1	0	-2.525502	2.561361	1.033451
10	1	0	-1.166852	3.691334	0.976292
11	7	0	0.398038	1.681543	-3.122017
12	7	0	-1.068231	2.327159	2.542673
13	1	0	-0.620486	1.590639	-3.160103
14	6	0	0.984400	0.705359	-4.076027
15	1	0	0.615560	0.933348	-5.071399
16	1	0	2.065915	0.808628	-4.038263
17	1	0	0.686641	-0.295757	-3.779240
18	6	0	0.744920	3.073778	-3.511776
19	1	0	1.816705	3.201168	-3.380355
20	1	0	0.469295	3.215094	-4.552445
21	1	0	0.197166	3.769455	-2.885130
22	6	0	-1.514843	0.983550	2.892095
23	1	0	-1.302933	0.794606	3.943241
24	1	0	-2.595544	0.858371	2.728749
25	1	0	-0.987669	0.235901	2.302995
26	6	0	-1.723975	3.285687	3.423633
27	1	0	-2.819266	3.238890	3.333336
28	1	0	-1.457871	3.078673	4.458998
29	1	0	-1.403182	4.297253	3.178247

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PES_I-1.log
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.764811	-1.054558	-0.189736
2	1	0	-1.167413	0.630169	-1.165332
3	6	0	1.378663	0.244360	0.051007
4	6	0	-1.563328	0.132879	-0.252332
5	1	0	1.312076	0.786884	-0.891404
6	1	0	0.965612	0.859576	0.847458
7	1	0	-1.227007	0.827593	0.545502
8	1	0	-1.248142	-2.023821	-0.292816
9	7	0	2.830746	0.084766	0.353075
10	7	0	-2.989335	-0.050187	-0.322443
11	1	0	2.914201	-0.384953	1.259426
12	6	0	3.466416	1.426312	0.479458
13	1	0	4.508105	1.285585	0.749309

14	1	0	3.385131	1.923896	-0.483475
15	1	0	2.944626	1.988558	1.247626
16	6	0	3.551997	-0.741150	-0.653401
17	1	0	3.380062	-0.301422	-1.632863
18	1	0	4.608985	-0.722407	-0.407018
19	1	0	3.185222	-1.761161	-0.616276
20	6	0	-3.614905	1.249690	-0.573769
21	1	0	-4.693795	1.123378	-0.624987
22	1	0	-3.384247	1.968431	0.222757
23	1	0	-3.264991	1.654244	-1.521857
24	6	0	-3.475578	-0.581959	0.953156
25	1	0	-3.260503	0.103375	1.783070
26	1	0	-4.551118	-0.730932	0.891980
27	1	0	-3.011396	-1.544865	1.164675
28	6	0	0.663778	-1.085494	-0.034819
29	1	0	1.018755	-1.739019	-0.847146
30	1	0	0.821826	-1.722869	0.856164

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PES_I1.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.886071	-0.845800	-0.308636
2	1	0	0.484953	-0.810628	-1.314546
3	6	0	-1.181948	-0.149701	1.008558
4	6	0	2.327086	-1.160851	-0.207673
5	1	0	-1.921356	-0.532941	1.709118
6	1	0	-0.765257	0.770743	1.411485
7	1	0	2.886050	-1.393348	-1.101498
8	1	0	2.697323	-1.560843	0.725425
9	7	0	-1.938086	0.242780	-0.222888
10	7	0	1.883681	0.241308	-0.115768
11	1	0	-1.279277	0.649523	-0.892673
12	6	0	-2.930336	1.301655	0.107670
13	1	0	-3.423179	1.609869	-0.809195
14	1	0	-3.650075	0.879599	0.804411
15	1	0	-2.407581	2.138902	0.560149
16	6	0	-2.601712	-0.911324	-0.884868
17	1	0	-3.248246	-1.389998	-0.153554
18	1	0	-3.184391	-0.532290	-1.718865
19	1	0	-1.850584	-1.605969	-1.246899
20	6	0	2.142946	1.116146	-1.274265
21	1	0	1.404829	1.914765	-1.269176
22	1	0	3.146239	1.522856	-1.173821
23	1	0	2.063575	0.531536	-2.185756
24	6	0	2.019667	0.938632	1.176899
25	1	0	3.044808	1.292304	1.252653
26	1	0	1.333663	1.781712	1.187492
27	1	0	1.806508	0.258239	1.993628

28	6	0	-0.098699	-1.189692	0.773637
29	1	0	0.403986	-1.348943	1.726175
30	1	0	-0.538407	-2.148811	0.498352

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432930	1.521589	-0.573631
2	1	0	-0.145907	0.965505	-1.462451
3	6	0	1.324992	0.484512	0.978651
4	6	0	-1.550657	0.907282	0.175561
5	1	0	2.200924	0.709165	1.585096
6	1	0	0.588284	-0.016361	1.606304
7	1	0	-0.795880	2.498096	-0.904297
8	1	0	-1.871617	1.429443	1.072114
9	7	0	1.769968	-0.532456	-0.029828
10	7	0	-2.180006	-0.172790	-0.087239
11	1	0	0.957016	-0.817737	-0.583665
12	6	0	2.275290	-1.750255	0.658957
13	1	0	2.517599	-2.494841	-0.092883
14	1	0	3.163248	-1.473552	1.221522
15	1	0	1.501225	-2.118637	1.325475
16	6	0	2.790005	0.003067	-0.969621
17	1	0	3.610225	0.404660	-0.379387
18	1	0	3.135789	-0.813220	-1.596350
19	1	0	2.343604	0.777684	-1.584451
20	6	0	-1.933488	-1.050286	-1.233301
21	1	0	-1.740551	-2.049232	-0.848165
22	1	0	-2.836852	-1.069362	-1.839186
23	1	0	-1.096276	-0.707451	-1.826145
24	6	0	-3.258139	-0.649953	0.786110
25	1	0	-4.162911	-0.745321	0.190405
26	1	0	-2.973697	-1.626845	1.170377
27	1	0	-3.408705	0.050851	1.599644
28	6	0	0.760688	1.752568	0.365790
29	1	0	0.449145	2.383437	1.198652
30	1	0	1.530150	2.298948	-0.175752

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PES_I2.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.409111	0.117798	-0.524534
2	1	0	-0.489848	-0.845170	-1.026258
3	6	0	1.688884	-0.713822	0.642683

4	6	0	-1.742985	0.712375	-0.283479
5	1	0	2.205363	-0.780334	1.598842
6	1	0	1.568708	-1.715192	0.232956
7	1	0	0.120705	0.808168	-1.183311
8	1	0	-1.835544	1.791789	-0.238129
9	7	0	2.625088	0.002559	-0.282533
10	7	0	-2.817648	0.048210	-0.101028
11	1	0	2.209444	0.008885	-1.217662
12	6	0	3.911551	-0.737912	-0.382786
13	1	0	4.529167	-0.252217	-1.131874
14	1	0	4.393930	-0.702351	0.590472
15	1	0	3.699375	-1.763963	-0.667841
16	6	0	2.857865	1.414919	0.117736
17	1	0	3.207738	1.418512	1.147031
18	1	0	3.609670	1.836644	-0.542479
19	1	0	1.931145	1.971975	0.025277
20	6	0	-2.879132	-1.418226	-0.103346
21	1	0	-3.657911	-1.715929	0.592105
22	1	0	-3.137884	-1.759679	-1.103661
23	1	0	-1.931084	-1.839891	0.209299
24	6	0	-4.107206	0.716373	0.092822
25	1	0	-4.797036	0.341639	-0.660632
26	1	0	-4.483908	0.462526	1.080658
27	1	0	-3.979780	1.788469	-0.006358
28	6	0	0.343153	-0.035901	0.809058
29	1	0	-0.238090	-0.673596	1.476585
30	1	0	0.445644	0.930719	1.300977

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PES_TS-1.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.729537	-0.359210	-0.455963
2	1	0	-1.124327	-1.046794	-1.199904
3	6	0	1.030354	0.146736	1.280503
4	6	0	-1.553672	0.706762	-0.053515
5	1	0	1.218299	1.184945	1.010959
6	1	0	0.290120	0.111713	2.078266
7	1	0	-1.075142	1.516259	0.510093
8	1	0	-1.856867	-0.043104	0.777405
9	7	0	2.297837	-0.388919	1.853688
10	7	0	-2.685327	1.049111	-0.853616
11	1	0	2.137461	-1.371043	2.096805
12	6	0	2.641676	0.331655	3.111110
13	1	0	3.530627	-0.127690	3.531772
14	1	0	2.831005	1.371980	2.859661
15	1	0	1.805753	0.249324	3.799068
16	6	0	3.432816	-0.335969	0.892715
17	1	0	3.548619	0.695865	0.570575

18	1	0	4.324967	-0.678367	1.407320
19	1	0	3.225553	-0.983290	0.047254
20	6	0	-2.225896	1.829959	-2.008755
21	1	0	-3.087186	2.089980	-2.619763
22	1	0	-1.721953	2.753092	-1.698225
23	1	0	-1.540325	1.234878	-2.609913
24	6	0	-3.618018	1.844240	-0.052034
25	1	0	-3.153251	2.770203	0.307398
26	1	0	-4.480083	2.100636	-0.663169
27	1	0	-3.956182	1.264007	0.804483
28	6	0	0.573684	-0.679193	0.095185
29	1	0	1.212096	-0.525767	-0.795689
30	1	0	0.628210	-1.756679	0.280710

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PES_TS1.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.699800	0.425470	-0.555326
2	1	0	0.750834	0.073701	-1.584783
3	6	0	-1.579524	-0.358345	-0.285878
4	6	0	1.902454	0.585029	0.166402
5	1	0	-1.774192	-0.489288	-1.348572
6	1	0	-1.190274	-1.284388	0.129515
7	1	0	1.767764	0.614525	1.256697
8	1	0	1.885931	1.693097	-0.114691
9	7	0	-2.888094	-0.112797	0.378744
10	7	0	3.085188	-0.049864	-0.325910
11	1	0	-2.714355	-0.024810	1.384587
12	6	0	-3.779874	-1.288572	0.175476
13	1	0	-4.692077	-1.123455	0.739669
14	1	0	-3.995809	-1.363542	-0.887046
15	1	0	-3.266892	-2.178438	0.527091
16	6	0	-3.553782	1.135678	-0.080044
17	1	0	-3.643146	1.089949	-1.162507
18	1	0	-4.535525	1.178964	0.380926
19	1	0	-2.967879	1.995884	0.226277
20	6	0	2.986550	-1.490237	-0.063706
21	1	0	3.890268	-1.977093	-0.422508
22	1	0	2.875056	-1.698294	1.007629
23	1	0	2.132491	-1.908162	-0.595384
24	6	0	4.252133	0.498536	0.367772
25	1	0	4.191949	0.335000	1.450698
26	1	0	5.148971	0.011512	-0.007390
27	1	0	4.329316	1.567279	0.177504
28	6	0	-0.608648	0.804983	-0.039165
29	1	0	-0.920939	1.662365	-0.651796
30	1	0	-0.565813	1.088573	1.011063

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PES_TS2.log
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.635896	-0.254993	0.280732
2	1	0	-1.028376	0.609563	0.814819
3	6	0	1.685388	0.772092	0.416482
4	6	0	-1.636432	-0.804080	-0.665356
5	1	0	2.592197	0.986700	-0.146768
6	1	0	1.306391	1.697798	0.845603
7	1	0	-0.429539	-1.041353	1.007062
8	1	0	-1.681516	-1.877609	-0.810525
9	7	0	2.109950	-0.078570	1.574528
10	7	0	-2.449076	-0.115543	-1.369936
11	1	0	1.295250	-0.227352	2.175195
12	6	0	3.125754	0.643843	2.387238
13	1	0	3.370562	0.036792	3.253281
14	1	0	4.005153	0.794865	1.766806
15	1	0	2.708079	1.597676	2.695326
16	6	0	2.617743	-1.410423	1.152700
17	1	0	3.427651	-1.251235	0.444726
18	1	0	2.980125	-1.931005	2.033871
19	1	0	1.812548	-1.975854	0.694594
20	6	0	-2.525559	1.346186	-1.369870
21	1	0	-2.233603	1.693282	-2.359072
22	1	0	-3.558689	1.628833	-1.182064
23	1	0	-1.876063	1.775350	-0.617907
24	6	0	-3.389993	-0.756924	-2.294154
25	1	0	-4.400479	-0.507921	-1.978346
26	1	0	-3.216697	-0.358225	-3.290864
27	1	0	-3.239503	-1.830596	-2.279673
28	6	0	0.645178	0.128567	-0.478651
29	1	0	0.406242	0.867266	-1.244610
30	1	0	1.053471	-0.739756	-0.994578

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PES_(Z)-Me4-H+.log
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.256056	1.980933	-0.537131
2	6	0	-0.998597	1.820146	-0.126510
3	1	0	0.473627	2.693058	-1.322925
4	1	0	-1.777247	2.413193	-0.591141
5	6	0	1.416555	1.208588	0.027415
6	6	0	-1.414574	0.845366	0.945903
7	1	0	2.369446	1.575793	-0.349027

8	1	0	1.425889	1.262566	1.116766
9	1	0	-2.458297	1.020513	1.230604
10	1	0	-0.799646	0.996420	1.836849
11	7	0	1.331768	-0.245173	-0.315352
12	7	0	-1.236696	-0.556552	0.528871
13	1	0	0.342603	-0.535850	-0.005801
14	6	0	2.316868	-1.035959	0.450033
15	1	0	2.204108	-2.083568	0.183900
16	1	0	3.319239	-0.693267	0.199578
17	1	0	2.128372	-0.898763	1.511782
18	6	0	1.451949	-0.485447	-1.768986
19	1	0	2.438963	-0.165754	-2.098547
20	1	0	1.321114	-1.548051	-1.955684
21	1	0	0.682117	0.078405	-2.289227
22	6	0	-2.133948	-0.896570	-0.572688
23	1	0	-1.954694	-1.925950	-0.879890
24	1	0	-3.185182	-0.795136	-0.274468
25	1	0	-1.947216	-0.241173	-1.422950
26	6	0	-1.443585	-1.452841	1.661604
27	1	0	-2.458073	-1.357500	2.068673
28	1	0	-1.293267	-2.482887	1.341110
29	1	0	-0.727169	-1.221960	2.449556

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(Z)-H2Et2-2H+.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.137981	-2.284364	0.694815
2	1	0	1.094782	-2.520547	0.195689
3	6	0	-0.629772	-1.390144	0.333533
4	6	0	0.677675	-1.521639	0.065664
5	6	0	-1.496802	-0.161104	0.246196
6	6	0	1.651160	-0.488027	-0.439005
7	1	0	-1.030985	0.679618	-0.270787
8	1	0	-1.800531	0.168528	1.243828
9	1	0	1.941300	-0.700507	-1.473900
10	1	0	1.280489	0.535304	-0.385664
11	7	0	-2.781866	-0.467400	-0.506936
12	7	0	2.941284	-0.533141	0.364974
13	1	0	-2.544289	-0.812612	-1.443849
14	1	0	-3.268568	-1.242882	-0.040728
15	1	0	3.284685	-1.500576	0.381831
16	1	0	2.741687	-0.293010	1.343452
17	6	0	-3.775490	0.698387	-0.651106
18	6	0	4.083432	0.364987	-0.137960
19	1	0	-4.528500	0.339517	-1.357174
20	1	0	-3.218739	1.512349	-1.121690
21	1	0	4.956662	0.064058	0.446212
22	1	0	4.249214	0.082817	-1.180520

23	6	0	-4.398743	1.098335	0.675890
24	6	0	3.780269	1.843931	0.032507
25	1	0	-5.153612	1.864366	0.475699
26	1	0	-3.680498	1.533982	1.375044
27	1	0	-4.914143	0.260302	1.157129
28	1	0	4.669818	2.406861	-0.264572
29	1	0	2.959338	2.188614	-0.601792
30	1	0	3.572223	2.103097	1.076224

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(Z)-H2Et2-H+.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.503826	2.290420	-0.143822
2	6	0	0.824303	2.247617	-0.339739
3	1	0	-0.993147	3.236809	-0.359600
4	1	0	1.269629	3.166134	-0.718759
5	6	0	-1.459060	1.225719	0.345880
6	6	0	1.853535	1.158663	-0.151918
7	1	0	-1.452632	1.134956	1.438401
8	1	0	-2.476960	1.479663	0.046064
9	1	0	2.753042	1.622780	0.273527
10	1	0	2.154827	0.784326	-1.140506
11	7	0	-1.123195	-0.136764	-0.193702
12	7	0	1.411764	-0.001898	0.653354
13	6	0	-1.997540	-1.271773	0.271546
14	1	0	-1.951252	-1.273255	1.364215
15	1	0	-1.516614	-2.186817	-0.085275
16	6	0	-3.433377	-1.181228	-0.231212
17	1	0	-1.137072	-0.093345	-1.216714
18	6	0	2.325509	-1.178076	0.589898
19	1	0	1.839279	-1.982704	1.151789
20	1	0	2.366462	-1.497668	-0.457766
21	6	0	3.735229	-0.943800	1.134397
22	1	0	1.349059	0.295286	1.628630
23	1	0	-0.072941	-0.282172	0.124004
24	1	0	4.301538	-1.879457	1.104560
25	1	0	4.291754	-0.206431	0.548682
26	1	0	3.707724	-0.608179	2.177363
27	1	0	-3.976745	-2.076133	0.084002
28	1	0	-3.966367	-0.317158	0.173747
29	1	0	-3.475363	-1.141258	-1.325131

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(Z)-Me4-2H+.log

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	1.153405	-0.071780	-2.079579
2	1	0	-1.153360	-0.071745	-2.079601
3	6	0	0.670078	-0.286143	-1.126399
4	6	0	-0.670058	-0.286123	-1.126412
5	6	0	1.588707	-0.689622	-0.001969
6	1	0	1.800104	-1.763841	-0.051136
7	1	0	1.189254	-0.470251	0.992237
8	6	0	-1.588720	-0.689575	-0.001998
9	1	0	-1.189285	-0.470203	0.992214
10	1	0	-1.800134	-1.763792	-0.051161
11	7	0	2.940659	0.002920	-0.085426
12	7	0	-2.940658	0.002987	-0.085492
13	1	0	3.299545	-0.150702	-1.034932
14	1	0	-3.299527	-0.150641	-1.035004
15	6	0	3.942866	-0.623387	0.860322
16	1	0	4.902210	-0.121894	0.730581
17	1	0	3.587240	-0.489985	1.882710
18	1	0	4.040142	-1.683639	0.624770
19	6	0	2.852001	1.496178	0.118684
20	1	0	3.839249	1.929504	-0.044214
21	1	0	2.139635	1.915311	-0.591666
22	1	0	2.528217	1.684444	1.143245
23	6	0	-3.942896	-0.623291	0.860242
24	1	0	-4.040165	-1.683550	0.624721
25	1	0	-3.587304	-0.489855	1.882638
26	1	0	-4.902236	-0.121801	0.730453
27	6	0	-2.851983	1.496247	0.118604
28	1	0	-3.839225	1.929582	-0.044305
29	1	0	-2.528204	1.684520	1.143165
30	1	0	-2.139608	1.915366	-0.591746

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(Z)-Me4-H+.log
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632949	1.974926	-0.143241
2	6	0	0.708079	1.945505	-0.107731
3	1	0	-1.153279	2.836463	0.265963
4	1	0	1.225275	2.794067	0.333253
5	6	0	-1.490843	0.889847	-0.749077
6	6	0	1.567398	0.823654	-0.653663
7	1	0	-2.545052	1.176428	-0.778289
8	1	0	-1.174188	0.664521	-1.772845
9	1	0	2.627875	1.110306	-0.618124
10	1	0	1.321680	0.654031	-1.709840
11	7	0	-1.392656	-0.419425	0.013847
12	7	0	1.360964	-0.469936	0.058872
13	6	0	-1.966609	-0.314012	1.390446

14	1	0	-1.483969	0.508920	1.916976
15	1	0	-1.785548	-1.248930	1.922542
16	1	0	-3.041610	-0.132268	1.322231
17	6	0	-2.009828	-1.548036	-0.746052
18	1	0	-3.073713	-1.351264	-0.896086
19	1	0	-1.514378	-1.644673	-1.713092
20	1	0	-1.885325	-2.470491	-0.177074
21	6	0	1.888847	-0.400672	1.438828
22	1	0	1.400713	0.408497	1.987347
23	1	0	1.691458	-1.344486	1.953500
24	1	0	2.973807	-0.221579	1.446243
25	6	0	2.014264	-1.571988	-0.678046
26	1	0	1.837534	-2.515037	-0.154655
27	1	0	3.100148	-1.420455	-0.760369
28	1	0	1.598561	-1.646046	-1.686830
29	1	0	-0.316391	-0.591709	0.095382
