Reversible photoreduction as a new trigger for photoresponsive gels

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SUPPORTING INFORMATION

Instruments and Procedures

Hydrogel Formation

A pH switch method was used to form the hydrogels. 10 mg of gelator **1** was dissolved using 1 molar equivalent of 0.1 M sodium hydroxide. This was then topped up with water to give 2 mL of solution and a concentration of 5 mg/mL of gelator in solution. The solution was stirred until all the gelator was dissolved. This solution was then transferred to a vial containing a 6 mg of glucono-δ-lactone (GdL) and shaken gently. 1 mL was then transferred to a 20 mL plastic syringe with the top removed. The open syringe was covered with Parafilm and the solution was left to gel overnight. The gel was removed from the syringe by pushing the plunger.

Rheological Measurements

Dynamic rheological measurements were performed using an Anton Paar Physica MCR101 rheometer. A parallel measuring system was used to perform all tests. For strain tests the gels were prepared as described above and transferred onto the bottom plate for measurement. All experiments were performed at 25 °C.

Frequency sweeps: Frequency sweeps were performed with a 25 mm plate with a plate gap of 1.3 mm. Tests were performed at a strain of 0.5 % from 1 to 100 rad/s.

Strain sweep: Strain sweeps were performed with a 25 mm plate from 0.1 % to 100 % with a frequency of 10 rad/s, with a gap of 1.3 mm. The critical strain was quoted as the point that G' starts to deviate for linearity and ultimately crosses over the G", resulting in gel breakdown.

Dynamic Nanoindentation

Dynamic nanoindentation was performed using a Keysight Technologies Nanoindenter G200 with a DCM-II Head. Measurements were conducted with a 100 μm flat punch indenter (Synton-MDP Ltd, Nidau, Switzerland) at room temperature (25°C). The sample was placed in a custom sample holder (20 mm diameter, with a 5mm well) and 10 indentations were made on the sample (5 x 2 array) with 400 μm spacing between each indent. The tip was

cleaned after each indent to prevent any of the gel material being transferred to the subsequent indent by indenting a piece of double-sided Scotch tape (3M, Bracknell, UK) which was mounted on an adjacent sample puck. The refined surface detection methodology that we employed in our previous studies was used for testing.[1] A pre-compression of 5 μm was applied to the samples. The testing frequency was 15 Hz. Immediately after completion of the indentations, the gel was kept in the sample puck and the side of the gel that had been indented was masked. It was then irradiated for 30 minutes (as described below). The irradiated side was subsequently indented using the same approach as described above i.e. 10 indents (5 x 2) with 400 μm spacing.

SEM Imaging

SEM images were obtained using a Hitachi S-4800 FE-SEM at 3 keV. The gel was deposited onto glass cover slips which were fixed onto aluminium SEM stubs with carbon tabs and left to dry for 24 hours. The samples were gold coated for 3 minutes at 15 mA prior to imaging using a sputter coater (EMITECH K550X).

Irradiating Samples

Gels were placed onto a glass microscope slide and placed inside a plastic petri dish with a wet paper towel in to keep the air saturated with water and to prevent the gel drying out. The lid of the petri dish had a hole cut out to allow the LED to be able to irradiate the sample. A heat filter was then placed over this hole to prevent sample from heating up. A 365 nm LED or 490 nm LED (LedEngin Inc, LZ1-10U600) with a light source powered by a TTi QL564P power supply operating at 1.0 W was used to irradiate gel samples. When using a mask a shape was cut out of a sheet of opaque plastic and placed over the sample prior to irradiation.

Sealing samples

Samples were left to recover on a glass slide before being photographed or for rheological measurements. They were then placed in a petri dish with a

wet paper towel to ensure the atmosphere was saturated with water. The petri dish was then sealed with Parafilm and the sample was kept at room temperature and out of direct sunlight.

UV-vis absorption measurements

Measurements were carried out on a Shimadzu UV-2550 UV−Vis spectrophotometer running the UV Probe software, version 2.34 using the integrated sphere accessory with a slit width of 5 nm and collecting data 1 nm per second. Gel samples for UV-vis absorptions were performed as mentioned above, but placed in a demountable 0.1 mm quartz cuvette. Solution samples were also placed in a 0.1 mm demountable cuvette. Samples were irradiated with a 365 nm LED or a 490 nm LED for 5 minutes and the spectra collected. Kinetic measurements were collected for 16 hours measuring the absorbance at 720 nm every 15 minutes.

Electron paramagnetic resonance (EPR)

Samples were prepared for EPR measurements by loading 30 μL of a solution of 1 to which GdL had been added into a glass capillary with an internal diameter 1.0 mm. Dilutions were prepared by diluting the initial solution of **1**. The capillaries were stored overnight before measurement. For the samples where SDS was added, **1** (1.18 mg) was dissolved into 10 mM SDS in 0.1 M NaOH solution (236 μL). This was then loaded into glass capillary.

Background measurements were taken for all samples by recording spectrum before exposure to UV. No EPR signal was seen in any background measurement. The samples were then exposed to UV light outside the EPR cavity for up to 60 seconds, before being placed in the spectrometer and a spectrum recorded. EPR Parameters: Microwave Power = 1 mW, Sweep Time = 60 s, Sweep width = 150 G, Modulation frequency = 100 kHz, Modulation width = 1 G, Time constant = 0.1 s.

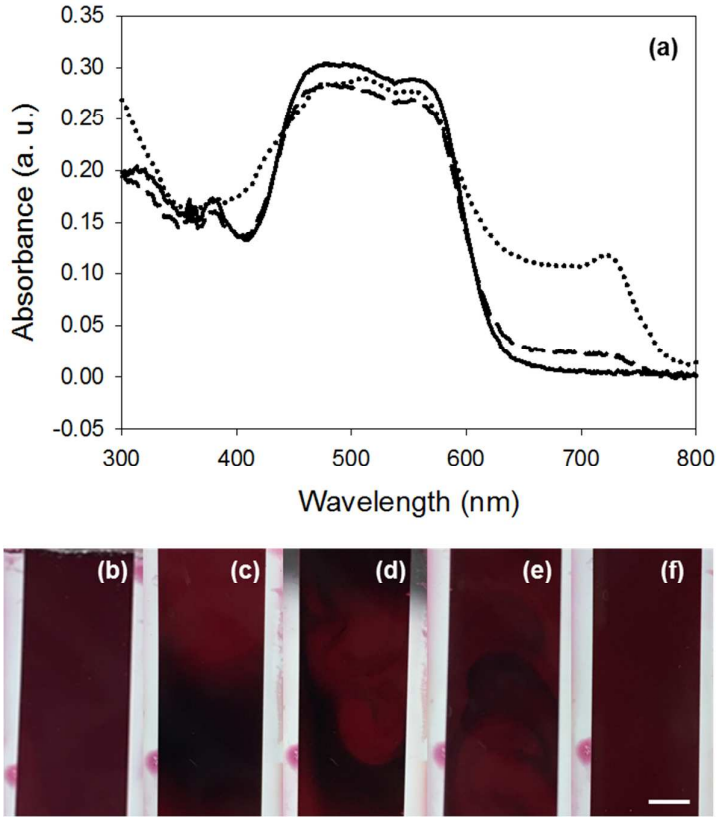

Figure S1 (a) UV-vis absorption spectra of a solution of 1 at 5 mg/mL before irradiation (dashed line), immediately after irradiation with a 365 nm LED for 10 minutes (dotted line) and the solid data show the decrease in the presence of the radical anion overtime; Photographs of a solution of 1 in a 1 mm quartz cuvette (b) before irradiation, (c) immediately after irradiation, (d) 5 minutes after irradiation, (e) 10 minutes after irradiation and (f) 20 minutes after irradiation. The scale bar represents 0.5 cm.

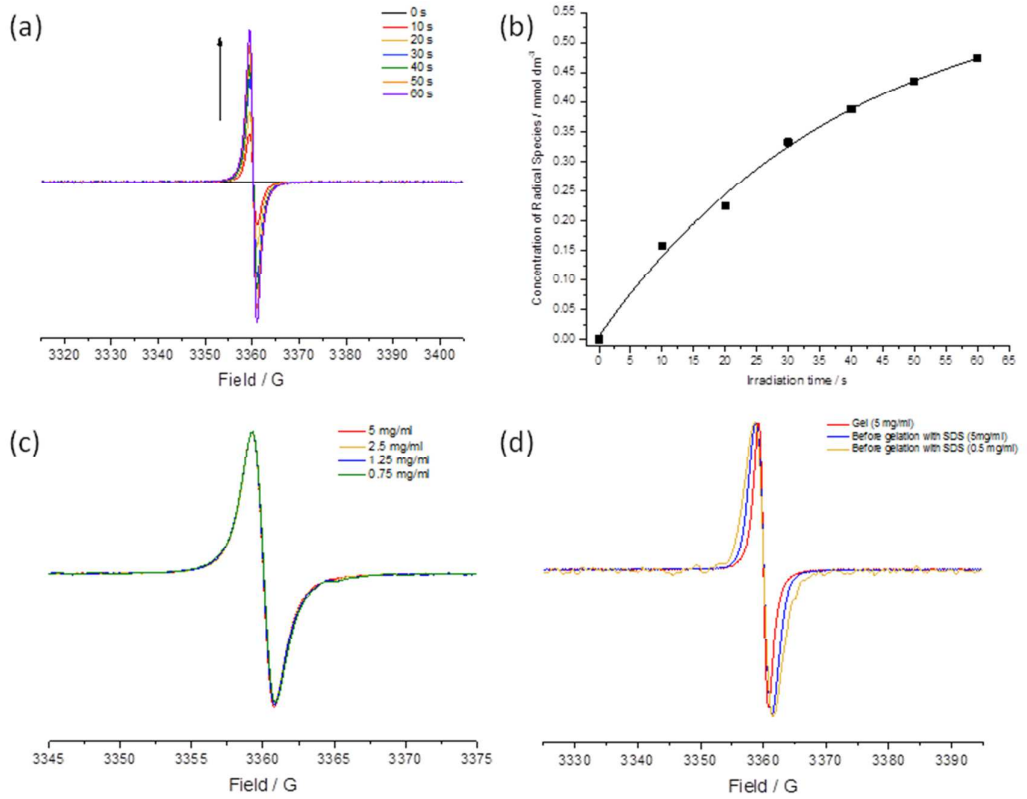

Figure S2 (a) EPR measurements taken every 10 seconds. The radical signal increased significantly over short exposure time. (b) Radical concentration for different exposure times was calculated by comparing 2nd integrals of spectra to an amino-TEMPO standard at 10^{-4} mol/dm^3 in water. (c) Spectra recorded after 60 s exposure to UV light for a range of samples of **1** at pH 4 at different concentrations. Signals were normalised and line shapes were compared. No significant change in the line shape and no significant broadening were observed. This would be expected if gel fibres do not change with concentration and have similar density. (d) Adding a surfactant (SDS) to a sample of **1** at high pH was carried out in an attempt to achieve monomeric conditions,[2] therefore allowing calculation of the number of interaction sites in samples.

Regarding Figure S2d, some broadening of lines was observed upon addition of surfactant, suggesting that the aggregates of **1** at high pH are disrupted and exchange interactions/electron hopping are less significant. We interpret this as the competing SDS micelle formation may lead to a breakdown in aggregates of **1**; therefore separating radical centres formed upon irradiation,

leading to a more monomer-like character. Further dilution of SDS containing solution was performed, decreasing the concentration of **1** by a factor of 10 compared to [SDS], therefore driving radical centres further apart. This gave further broadening of the line, indicating a further reduction in exchange interactions/electron hopping. The line shape of diluted sample changed to a more Gaussian (around 40% Lorentzian, pseudo Voigt) compared to around 75% Lorentzian for the gel at a concentration of **1** of 5 mg/mL. This suggests a significant reduction in homogenous broadening as compared to inhomogeneous broadening, however it is clear that even under these conditions there is still a significant Lorentzian contribution, and therefore it is unlikely that we are able to achieve monomer conditions. Hence it is not possible from these experiments to exactly determine the number of interaction sites between radicals. However it is clear that upon dilution of sample or addition of surfactant there is a change in exchange interactions/electron hopping.

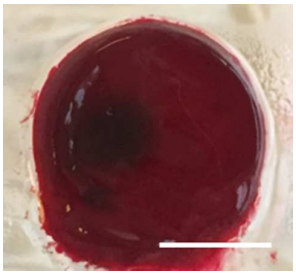

Figure S3 Photograph of a gel of 1 photographed 24 hours after being irradiated. Scale bar represents 1 cm.

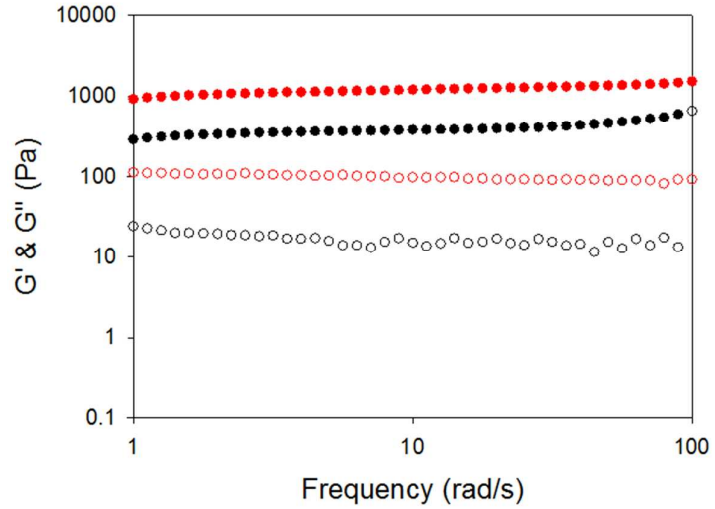

Figure S4 Frequency sweeps performed on gels of 1 (black data) compared to gels of 1 irradiated with a 365 nm LED for 1 hour (red data) performed at 10 rad/s at 25 °C; Full symbols are G' and empty symbols are G".

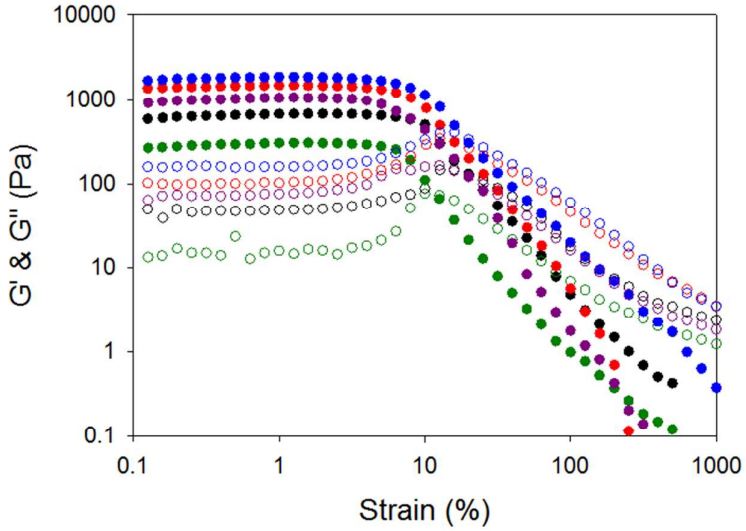

Figure S5 Rheological tests performed on gels of 1 with increasing times of irradiation with a 365 nm LED. Green data is 0 minutes, black data is 15 minutes, purple data is 30 minutes, red data is an hour and blue data is 2 hours strain sweeps performed at 10 rad/s at 25 °C. Full symbols are G' and open symbols are G".

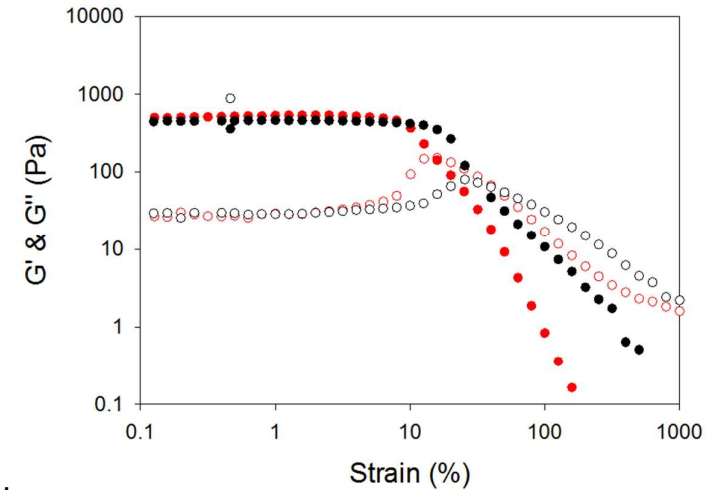

Figure S6 Rheological tests performed on gels of **1** irradiated for an hour and left to recover overnight (black data) compared to a gel that has not been irradiated (red data). Strain sweeps performed at 10 rad/s at 25 °C. Full symbols are G' and empty symbols are G".

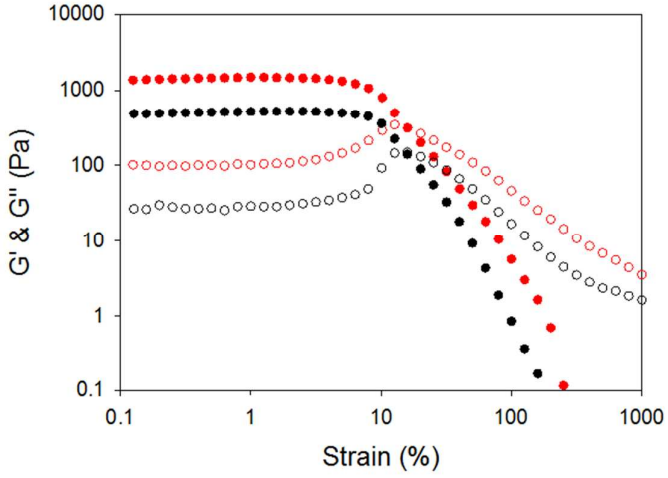

Figure S7 Rheological tests performed on gels of **1** sealed in a hydrated chamber for an hour (black data) compared to gels of **1** irradiated with a 365 nm LED for 1 hour (red data). Full symbols are G' and empty symbols are G" strain sweeps performed at 10 rad/s at 25 °C.

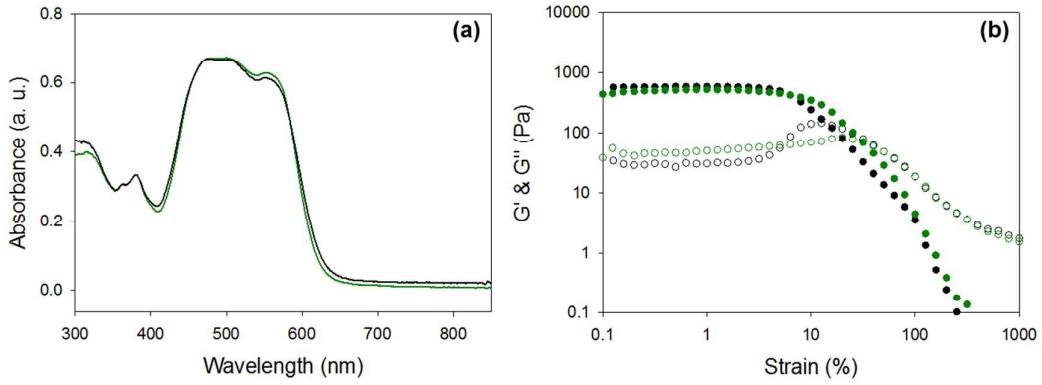

Figure S8 Comparing gels of **1** irradiated for an hour with 490 nm LED (green data) compared to a gel that has not been irradiated (black data). (a) Strain sweeps performed at 10 rad/s at 25 °C. Full symbols are G' and empty symbols are G". (b) UV-vis absorption spectra showing no formation of the radical anion.

Further Computational Information

The effect of forming the radical anion was studied computationally in a two-step procedure. First the structures of cluster models consisting of two or more molecules of **1** were optimised using DFT. In the second step, an excess electron was localised on the cluster models and their structures were re-optimised using the same computational setup. These calculations typically used the B3LYP[3, 4] hybrid density functional together with the D3 dispersion correction[5] (B3LYP+D), either a DZP[6] or def2-TZVP[7] basis-set and were performed using the Turbomole 6.6 code. Some calculations, finally, used the COSMO dielectric screening model[8] to model the effect of the fibres being present in an environment with a high relative dielectric permittivity such as water (ε_r = 80). XYZ coordinates of the optimized gas phase (ε_r = 1) structures of the different cluster models are given in an appendix to this supporting information.

As discussed in the main text of the paper, we found that stable structures of stacked molecules of **1** involves a spiral staircase motive, where every PBI molecule is rotated, perpendicular to the stacking direction, relative to the

molecule below it (see Fig. 4a in the main paper). The stacks are held together by amongst other things intermolecular hydrogen bonds involving the protons of the carboxylic acid groups of one PBI molecule and the carbonyl oxygen atoms of the next molecule in the stack. A similar rotated structure was previously predicted by DFT+D calculations for a simpler PBI dimer without hydrogen bonds.[9]

Table S1 *Binding energies of the different cluster models of the stacks in their neutral state ($E_{bind,neutral} = E_{stack} – n*E_{PBI}$) and containing the radical anion ($E_{bind,anion,} = E_{stack} – E_{PBI,anion} - (n-1)*E_{PBI}$), as well as the difference between the two ($\Delta E_{bind,anion-neutral} = E_{bind,anion} - E_{bind,neutral}$). All values in kJ/mol, def2-TZVP values, where available, are given in between parentheses.*

Environment	n	2	3
$\varepsilon_r = 1$	$E_{bind,neutral}$	-199 (-155)	-397
	$E_{bind,anion}$	-244 (-199)	-467
	$\Delta E_{bind,anion-neutral}$	-45 (-44)	-69
$\varepsilon_r = 80$	$E_{bind,neutral}$	-152 (-102)	-303
	$E_{bind,anion}$	-166 (-114)	-323
	$\Delta E_{bind,anion-neutral}$	-14 (-12)	-20

Localising an excess electron on the stack models results in a minor contraction of the intermolecular distances and the intermolecular binding energy becoming more negative ($E_{bind,anion} < E_{bind,neutral}$, see Table S1). Forming the radical anion thus stabilises the stacks and increases the intermolecular binding between the PBI molecules in the stack. The effect of the excess charge is smaller, but still very significant, in the case of cluster models embedded in water, which is probably related to the fact that the excess electron is more localised in this case.

Changing the basis-set from DZP to def2-TZVP is found to have as expected a large effect on the predicted binding energies of the stacks due to reduction

in the basis set superposition error but only a very minor effect on the predicted stabilisation of the stacks with a radical anion relative to the neutral stacks ($\Delta E_{bind,anion-neutral}$), giving us confidence in our results. Similarly, switching from B3LYP+D to the GGA density functional PBE+D3 is found to have a small effect on the predicted stabilisation, where tested.

Concentrating on the results for the cluster model with three molecules of **1** (see Fig. 4b in the main paper)**,** generating the radical anion clearly stabilises the stacks energetically. We believe this stabilisation to result for a large extent from the electrostatic interaction between the charge of the excess electron localised on the central PBI molecule (see Fig. 4d of the main paper) and the positive quadruple moments in the stacking direction (θ_{zz}) of adjacent PBI molecules. As such this stabilisation is an example of favourable anion-π interactions, previously observed in the context of gas phase anion-PBI complexes for PBI derivatives,[10] resulting from the fact that the traceless zz component of the quadruple of **1** and related PBIs is positive (B3LYP/DZP predicts a value of 22 for a molecule of **1** in the gas phase).

Calculations on the same cluster model with three molecules of **1** but now with a charge of -2 rather than -1 shows that localization of two excess electrons near each other is energetically severely disfavored. In contrast to the stabilization, discussed above, for the localization of one excess electron on the stack, the dianion stacks are significantly destabilized relative to the neutral stacks, e.g. by +60 (triplet) and +77 kJ/mol (singlet) for B3LYP+D3/ DZP/ ε_r = 1. As discussed in the main paper this destabilization, most likely simply the result of the Coulombic repulsion between the charges of the two excess electrons, might be (part of) the explanation of why for long irradiation times the additional gain in rheological properties goes to zero (see Fig. S4 above).

The radical cation, finally, that for reasons of charge balance also must be formed, is predicted to have much smaller effect on the binding energies of the stack than its anion counterpart. B3LYP+D3/DZP calculations on the cluster with three molecules of **1** but now with a charge of +1 predict an

increase in the stack binding energy, relative to the neutral stack, for the low relative dielectric permittivity environment case (-26 kJ/mol rather than -69 kJ/mol) and effectively no change in the case of the stack embedded in water (+2 kJ/mol rather than -14 kJ/mol). Also, in contrast, to the anion the hole of the radical cation, or more correctly the unpaired electron left in the singly occupied molecular orbital after ionization of its partner, is not localized on one molecule but rather delocalized over the stack.

References

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Appendix - XYZ coordinates of DFT optimized gas phase cluster models and isolated molecules

PDI-valine - neutral (B3LYP+D3, DZP, grid 3, gas phase)

70
Energy = -2021.5963708850
C 2.3191354 1.3456951 1.5308785
C 1.7331400 2.3096355 2.3578310
C 0.7377476 3.1396206 1.8712033
C 0.3130416 3.0121815 0.5273014
C -0.7049285 3.8636528 0.0358724
C -1.1245066 3.7432625 -1.2779868
C -0.5500471 2.7861745 -2.1208043
C 0.4556017 1.9224944 -1.6804698
C 0.9051985 2.0297881 -0.3255405
C 1.9315429 1.1807494 0.1990263
C 2.5384853 0.1682661 -0.6772941
C 3.5416762 -0.6977479 -0.2359424
C 4.1108884 -1.6598458 -1.0766031
C 3.6905246 -1.7809809 -2.3901457
C 2.6780119 -0.9243296 -2.8838139
C 2.2520852 -1.0529843 -4.2272210
C 1.2608902 -0.2190002 -4.7155626
C 0.6774989 0.7474507 -3.8896837
C 1.0639109 0.9113080 -2.5573514
C 2.0882529 0.0603605 -2.0319607
H 3.0971418 0.7155367 1.9568803
H 2.0461833 2.4234771 3.3954499
C 0.1324714 4.1483291 2.7725682
C -1.3342273 4.8862020 0.9060510
H -1.9093266 4.4080217 -1.6380799
H -0.9120629 2.7282919 -3.1452458
H 3.9042649 -0.6393056 0.7882645
H 4.8912757 -2.3288196 -0.7146850
C 4.3120485 -2.8109307 -3.2571492
C 2.8501302 -2.0686473 -5.1256132
H 0.9469529 -0.3337058 -5.7528176
H -0.0983753 1.3796392 -4.3165692
N -0.8702307 4.9641049 2.2313986
C -1.5221087 5.9693681 3.0972837
O -2.2181868 5.6243350 0.5066126
O 0.4770861 4.2714942 3.9351331
N 3.8498265 -2.8872670 -4.5831786
O 5.1778042 -3.5663937 -2.8503355
O 2.4963983 -2.2006356 -6.2844680
C 4.4645983 -3.9281895 -5.4339857
C 4.7671190 -3.4046083 -6.8351567
C -2.7619038 5.4113576 3.8321223
C -3.6290275 6.5535027 4.3776026

H	-3.3429594	4.9141331	3.0364834
O	5.3494926	-2.1881347	-6.7776795
O	4.6279481	-4.0204760	-7.8612030
H	5.5192362	-1.9248928	-7.7009541
C	3.7146866	-5.2778014	-5.3651382
C	4.5892419	-6.4133447	-5.9127595
C	2.3293672	-5.2682440	-6.0183531
C	-0.5083923	6.7069656	3.9673925
H	5.4526721	-4.0893095	-4.9796354
H	3.5881147	-5.4581626	-4.2837676
C	-2.4444635	4.3771342	4.9162260
H	-1.8854444	6.7293217	2.3908150
O	0.5662128	7.0802843	3.2409448
O	-0.6719759	7.0312345	5.1161191
H	1.1601411	7.5484723	3.8562509
H	-3.8720995	7.2841952	3.5897640
H	-3.1177636	7.0805551	5.1937930
H	-4.5778961	6.1528076	4.7642563
H	4.7389851	-6.3078333	-6.9952653
H	4.1069318	-7.3836876	-5.7224103
H	5.5767911	-6.4306253	-5.4247893
H	2.4026005	-5.0201736	-7.0852014
H	1.6569921	-4.5389196	-5.5476826
H	1.8676838	-6.2626530	-5.9196332
H	-1.9294777	3.4975259	4.5080190
H	-3.3798156	4.0317926	5.3826653
H	-1.8042211	4.8119785	5.6947174

PDI-valine – anion (B3LYP+D3, DZP, grid 3, gas phase)

70
Energy = -2021.6932217990

C	2.3285029	1.3391246	1.5429224
C	1.7506602	2.2928410	2.3585979
C	0.7415619	3.1362230	1.8741702
C	0.3100677	3.0113122	0.5301723
C	-0.7111891	3.8592910	0.0344066
C	-1.1337576	3.7281577	-1.2955039
C	-0.5662686	2.7842858	-2.1296807
C	0.4577268	1.9109178	-1.6841860
C	0.9051180	2.0228871	-0.3277681
C	1.9328482	1.1707112	0.1919375
C	2.5296685	0.1720193	-0.6715049
C	3.5445811	-0.7100326	-0.2223449
C	4.1070673	-1.6586782	-1.0545036
C	3.6916919	-1.7829214	-2.3873467
C	2.6801528	-0.9256596	-2.8870236
C	2.2532454	-1.0461703	-4.2328868
C	1.2505159	-0.1967172	-4.7198969
C	0.6709727	0.7553663	-3.9035292
C	1.0598944	0.9173417	-2.5498029
C	2.0849999	0.0626595	-2.0290301
H	3.1086204	0.7060662	1.9608718
H	2.0632857	2.4125070	3.3960657
C	0.1504110	4.1311190	2.7631844
C	-1.3337419	4.8680749	0.8882337
H	-1.9218550	4.3928069	-1.6497171
H	-0.9251728	2.7187204	-3.1548410
H	3.8981084	-0.6496065	0.8049999
H	4.8859661	-2.3321086	-0.6965384
C	4.3082944	-2.7973341	-3.2388254
C	2.8433281	-2.0420414	-5.1214981
H	0.9432920	-0.3112403	-5.7595543
H	-0.1042474	1.3930948	-4.3234810
N	-0.8566430	4.9453293	2.2158386
C	-1.4987074	5.9470419	3.0780748
O	-2.2316287	5.6209150	0.5140853
O	0.4814886	4.2821335	3.9390377
N	3.8436127	-2.8627103	-4.5714618
O	5.1792769	-3.5758511	-2.8538280
O	2.5108800	-2.1943334	-6.2968007
C	4.4531917	-3.8954942	-5.4205988
C	4.7326104	-3.3847782	-6.8276851
C	-2.7492131	5.4006607	3.8040606
C	-3.6122258	6.5456128	4.3499295
H	-3.3266992	4.9131852	3.0006355
O	5.3448299	-2.1805831	-6.7940653
O	4.5780817	-4.0041921	-7.8540033

H	5.4650796	-1.9222282	-7.7254034
C	3.7153104	-5.2513692	-5.3393097
C	4.5880176	-6.3867401	-5.8898672
C	2.3224345	-5.2536346	-5.9759208
C	-0.4906178	6.6684339	3.9623921
H	5.4465919	-4.0517403	-4.9739076
H	3.6033993	-5.4240999	-4.2556792
C	-2.4488526	4.3583114	4.8849588
H	-1.8551437	6.7126904	2.3727242
O	0.5815043	7.0724181	3.2461050
O	-0.6547110	6.9854971	5.1171471
H	1.1777116	7.5004307	3.8863833
H	-3.8487421	7.2782702	3.5613174
H	-3.0974546	7.0697091	5.1665254
H	-4.5655603	6.1520886	4.7360573
H	4.7317052	-6.2807639	-6.9736802
H	4.1111809	-7.3603542	-5.6961703
H	5.5788580	-6.3988529	-5.4074626
H	2.3851641	-5.0268038	-7.0482880
H	1.6637459	-4.5064483	-5.5156427
H	1.8571580	-6.2447052	-5.8491064
H	-1.9161423	3.4905517	4.4760549
H	-3.3918043	4.0023672	5.3309420
H	-1.8234467	4.7900688	5.6773023

PDI-valine – cation (B3LYP+D3, DZP, grid 3, gas phase)

70
Energy = -2021.3261150250

C	0.7480781	3.6931094	-0.0472699
C	2.1377097	3.6805426	-0.0498453
C	2.8256124	2.4679501	-0.0446066
C	2.1087575	1.2521220	-0.0383978
C	2.8266736	0.0369919	-0.0338861
C	2.1397077	-1.1761843	-0.0303391
C	0.7499993	-1.1898691	-0.0315121
C	-0.0107500	0.0027320	-0.0350704
C	0.6820572	1.2515369	-0.0385846
C	-0.0116775	2.4998040	-0.0407473
C	-1.4617937	2.4991868	-0.0353684
C	-2.2225373	3.6917919	-0.0317205
C	-3.6122313	3.6781094	-0.0244875
C	-4.2991974	2.4649268	-0.0219855
C	-3.5812890	1.2497909	-0.0264067
C	-4.2981448	0.0339471	-0.0265110
C	-3.6102564	-1.1786577	-0.0312212
C	-2.2206283	-1.1912133	-0.0343085
C	-1.4608711	0.0021076	-0.0342568
C	-2.1546005	1.2503781	-0.0325634
H	0.2476168	4.6591122	-0.0506668
H	2.7115594	4.6068928	-0.0560762
C	4.3199377	2.4875814	-0.0463179
C	4.3217930	0.0199127	-0.0288667
H	2.7138122	-2.1023769	-0.0265572
H	0.2504100	-2.1563175	-0.0289104
H	-1.7229523	4.6582448	-0.0338344
H	-4.1863268	4.6043081	-0.0205716
C	-5.7942938	2.4820179	-0.0107766
C	-5.7924707	0.0142912	-0.0226954
H	-4.1841177	-2.1050207	-0.0326508
H	-1.7201717	-2.1572195	-0.0371311
N	4.9761489	1.2563167	-0.0282717
C	6.4635195	1.2217996	-0.0332867
O	4.9280060	-1.0323509	-0.0291791
O	4.9235701	3.5405445	-0.0638028
N	-6.4486353	1.2455981	-0.0050868
O	-6.4005184	3.5342682	-0.0107649
O	-6.3961283	-1.0387174	-0.0357275
C	-7.9360277	1.2801364	-0.0058565
C	-8.5159277	0.2452517	0.9595350
C	7.0535302	1.2071946	-1.4614714
C	8.5223036	0.7636838	-1.4293638
H	6.4864235	0.4149126	-1.9809418
O	-7.8379893	0.2508269	2.1263809
O	-9.5004066	-0.4137461	0.7611126

H	-8.2761513	-0.4003214	2.7066436
C	-8.5297584	1.2925922	-1.4325134
C	-9.9987576	1.7350872	-1.3973348
C	-8.3514024	-0.0182645	-2.2043258
C	7.0460292	2.2579959	0.9291137
H	-8.1750546	2.2493662	0.4535393
H	-7.9645349	2.0846307	-1.9544075
C	6.8742641	2.5172074	-2.2345107
H	6.7038000	0.2532253	0.4268357
O	6.3706369	2.2547420	2.0974582
O	8.0303959	2.9161768	0.7274555
H	6.8104531	2.9065896	2.6756802
H	8.6443332	-0.1876377	-0.8881221
H	9.1532456	1.5215782	-0.9476922
H	8.8865524	0.6115459	-2.4554348
H	-10.6280462	0.9771461	-0.9135919
H	-10.3654704	1.8861569	-2.4226867
H	-10.1202012	2.6867546	-0.8565697
H	-8.8360828	-0.8516325	-1.6793875
H	-7.2929199	-0.2754916	-2.3492807
H	-8.8070849	0.0773155	-3.2006889
H	5.8156453	2.7751161	-2.3771532
H	7.3274315	2.4199810	-3.2318628
H	7.3609187	3.3508473	-1.7118381

PDI-valine dimer - neutral (B3LYP+D3, DZP, grid 3, gas phase)

140
Energy = -4043.2685532560
C -1.4062583 0.4129098 1.9612199
C -2.3150987 1.4669480 1.8288887
C -2.9815110 1.6689388 0.6330154
C -2.7567835 0.7963678 -0.4559957
C -3.4662351 0.9961864 -1.6630567
C -3.2353546 0.1539793 -2.7384412
C -2.2927282 -0.8747237 -2.6428548
C -1.5610898 -1.0991384 -1.4746283
C -1.8090729 -0.2646597 -0.3401582
C -1.1243995 -0.4523272 0.9029939
C -0.1329904 -1.5287769 1.0131302
C 0.5624256 -1.7840518 2.1971551
C 1.5423451 -2.7779031 2.2787620
C 1.8617419 -3.5398852 1.1670633
C 1.1748686 -3.3221096 -0.0498966
C 1.5219023 -4.0848869 -1.1881360
C 0.8455308 -3.8928514 -2.3803864
C -0.1719845 -2.9373808 -2.4692547
C -0.5295537 -2.1397268 -1.3808757
C 0.1566164 -2.3256452 -0.1381068
H -0.8977317 0.2991443 2.9154686
H -2.4989465 2.1528560 2.6550524
C -3.8985425 2.8217799 0.5018810
C -4.4556272 2.0937615 -1.7999461
H -3.7985474 0.3148688 -3.6575351
H -2.1314169 -1.5021411 -3.5167708
H 0.3549479 -1.1972101 3.0892853
H 2.0766244 -2.9645605 3.2101307
C 2.9363122 -4.5575120 1.2727827
C 2.6419853 -5.0498935 -1.1369859
H 1.1321650 -4.4838657 -3.2493062
H -0.6659439 -2.8109064 -3.4298841
N -4.6262298 2.9364431 -0.6861541
C -5.5765871 4.0658917 -0.8350500
O -5.0892102 2.2692381 -2.8257212
O -4.0184438 3.6487973 1.3913601
N 3.2572261 -5.2641852 0.1002706
O 3.5299073 -4.7639825 2.3165542
O 3.0337361 -5.6301430 -2.1364981
C 4.4314261 -6.1688998 0.1596171
C 5.3831088 -5.8375652 -0.9934114
C -6.9844463 3.7519819 -0.2883264
C -7.9845067 4.8110593 -0.7716644
H -7.2585698 2.7963516 -0.7688129
O 5.5802523 -4.5061839 -1.0275564
O 5.9323977 -6.6255836 -1.7184133

C	4.0700072	-7.6551870	0.3557946
C	5.3233602	-8.4473825	0.7534256
C	3.3486481	-8.3121112	-0.8250844
C	-4.9278515	5.3623172	-0.3435531
H	4.9578231	-5.8466324	1.0682512
H	3.3878246	-7.6585868	1.2240667
C	-7.0584800	3.5647795	1.2303872
H	-5.6707802	4.1846960	-1.9228679
O	-3.7202694	5.4968893	-0.9208333
O	-5.4286441	6.1814003	0.3826742
H	-3.1790496	6.1468710	-0.4202438
C	2.2313289	1.1885185	1.5565631
C	1.6586072	2.1230373	2.4246881
C	0.7688344	3.0722669	1.9477599
C	0.4148820	3.0788851	0.5797363
C	-0.4764505	4.0666636	0.0930327
C	-0.8850527	4.0233899	-1.2304131
C	-0.4296670	3.0073105	-2.0789597
C	0.4766360	2.0364022	-1.6509018
C	0.9380353	2.0809677	-0.2978331
C	1.9019464	1.1486196	0.2001674
C	2.5156220	0.1914889	-0.7311179
C	3.5641528	-0.6530632	-0.3617263
C	4.1571569	-1.5415700	-1.2677067
C	3.6796626	-1.6415139	-2.5649968
C	2.5813184	-0.8421498	-2.9670083
C	2.0294070	-1.0130584	-4.2568415
C	0.9690535	-0.2194024	-4.6637630
C	0.4645899	0.7749538	-3.8205050
C	0.9734947	0.9747627	-2.5358584
C	2.0202570	0.1178940	-2.0713225
H	2.9366655	0.4693667	1.9676717
H	1.9031995	2.1263412	3.4868149
C	0.1636219	4.0375768	2.8937409
C	-0.9534942	5.1505129	0.9840941
H	-1.5891995	4.7659591	-1.5976183
H	-0.7963298	3.0006756	-3.1032659
H	3.9585467	-0.6256399	0.6518482
H	4.9783126	-2.1813387	-0.9501808
C	4.3323145	-2.5545733	-3.5330350
C	2.5396307	-2.0614701	-5.1689293
H	0.5455734	-0.3836380	-5.6544683
H	-0.3586443	1.3871728	-4.1824647
N	-0.6496665	5.0393220	2.3444888
C	-1.2619499	6.0495055	3.2406358
O	-1.5944408	6.1094046	0.5715097
O	0.3545374	3.9749739	4.0953876
N	3.6881955	-2.7538462	-4.7585298
O	5.3892329	-3.1247085	-3.2925259
O	2.0002955	-2.3181767	-6.2308504

C	4.2791433	-3.7762621	-5.6553752
C	4.2868277	-3.3198348	-7.1100934
C	-2.6618945	5.6240751	3.7353610
C	-3.4437536	6.8375627	4.2524541
H	-3.1773197	5.2667210	2.8323233
O	4.7047132	-2.0394555	-7.2128626
O	4.0718888	-4.0215157	-8.0647977
H	4.6993505	-1.8274221	-8.1645662
C	3.7217209	-5.1907078	-5.3846107
C	4.6689344	-6.2589533	-5.9436211
C	2.2817018	-5.4077513	-5.8579621
C	-0.2829415	6.5279813	4.3070390
H	5.3402888	-3.7899366	-5.3704645
H	3.7358624	-5.2895099	-4.2896342
C	-2.6524246	4.4806661	4.7534108
H	-1.4032255	6.9237827	2.5902142
H	5.9390521	-4.2357291	-1.9011036
O	0.9289764	6.7852677	3.7686041
O	-0.5586331	6.7685248	5.4542375
H	1.4906433	7.0985288	4.5014661
H	-7.9481771	4.9302439	-1.8662504
H	-7.7755314	5.7854123	-0.3099907
H	-9.0086940	4.5134020	-0.5024262
H	6.0369779	-8.4927094	-0.0803413
H	5.0481746	-9.4761397	1.0289737
H	5.8302228	-7.9936726	1.6199877
H	3.9605603	-8.2561836	-1.7343488
H	2.3841127	-7.8328003	-1.0371830
H	3.1538115	-9.3705811	-0.5935540
H	-6.4425683	2.7222283	1.5722238
H	-8.0985758	3.3583034	1.5258134
H	-6.7160933	4.4680943	1.7509601
H	-3.5064845	7.6254737	3.4854286
H	-2.9789285	7.2587220	5.1542443
H	-4.4731958	6.5387019	4.4987119
H	4.7271898	-6.2081610	-7.0395772
H	4.3095402	-7.2592230	-5.6608301
H	5.6825361	-6.1462680	-5.5278487
H	2.2073265	-5.3297695	-6.9506994
H	1.5906569	-4.6697497	-5.4289904
H	1.9427978	-6.4079995	-5.5490114
H	-2.1449055	3.5876881	4.3645009
H	-3.6877050	4.1984653	4.9964502
H	-2.1388209	4.7768185	5.6777875

PDI-valine dimer - anion (B3LYP+D3, DZP, grid 3, gas phase)

140
Energy = -4043.382624627

C	-1.2407599	0.3747794	1.8873176
C	-2.1265691	1.4372328	1.7349059
C	-2.7838220	1.6392305	0.5283871
C	-2.5537984	0.7616633	-0.5542400
C	-3.2383947	0.9669358	-1.7760824
C	-2.9837402	0.1256183	-2.8506192
C	-2.0670339	-0.9203082	-2.7337358
C	-1.3776204	-1.1679827	-1.5398174
C	-1.6248755	-0.3162779	-0.4175565
C	-0.9591058	-0.5064452	0.8344663
C	0.0013057	-1.5986502	0.9709448
C	0.7008770	-1.8337913	2.1633372
C	1.6300177	-2.8673517	2.2783261
C	1.9014099	-3.6989799	1.2002790
C	1.2248829	-3.4908976	-0.0263700
C	1.5366885	-4.3025454	-1.1390217
C	0.8801743	-4.1036409	-2.3468052
C	-0.0798132	-3.1021140	-2.4725403
C	-0.4054301	-2.2544171	-1.4065299
C	0.2573272	-2.4457454	-0.1519087
H	-0.7431837	0.2603314	2.8464676
H	-2.3080273	2.1350301	2.5510782
C	-3.6997988	2.7821390	0.3934364
C	-4.2186437	2.0639784	-1.9259074
H	-3.5145339	0.3026073	-3.7858505
H	-1.8883142	-1.5448927	-3.6057386
H	0.5312235	-1.1967374	3.0279862
H	2.1701827	-3.0345730	3.2101405
C	2.9421690	-4.7369125	1.3332952
C	2.6203201	-5.2950530	-1.0643677
H	1.1432717	-4.7296286	-3.1970166
H	-0.5520686	-2.9674222	-3.4430135
N	-4.4096244	2.8995414	-0.8089453
C	-5.3920809	3.9985766	-0.9507732
O	-4.8464379	2.2478093	-2.9587489
O	-3.8591451	3.5993342	1.2902525
N	3.2527571	-5.4732634	0.1733964
O	3.5398598	-4.9399284	2.3805285
O	2.9925197	-5.9282866	-2.0434816
C	4.4877587	-6.2896464	0.2103224
C	5.3839375	-5.8750948	-0.9651447
C	-6.8033108	3.5971708	-0.4745410
C	-7.8370376	4.6305467	-0.9412757
H	-7.0166902	2.6543049	-1.0080145
O	5.4550599	-4.5367273	-0.9973555
O	5.9874415	-6.6188684	-1.6982956

C	4.2598347	-7.7999585	0.4171798
C	5.5852997	-8.4764777	0.7959638
C	3.5829446	-8.5288017	-0.7475092
C	-4.8263881	5.3016201	-0.3738130
H	5.0042890	-5.9263488	1.1094540
H	3.5948609	-7.8587877	1.2967906
C	-6.9153660	3.3341738	1.0306729
H	-5.4489493	4.1613590	-2.0356450
O	-3.6233261	5.5309970	-0.9099882
O	-5.4030741	6.0520258	0.3759658
H	-3.0649582	6.1053790	-0.3230900
C	2.1267994	1.2732763	1.6177561
C	1.6021131	2.2291037	2.4749398
C	0.7604519	3.2377058	1.9974196
C	0.4124154	3.2669646	0.6262273
C	-0.4383462	4.2887846	0.1345712
C	-0.8005010	4.2872448	-1.2164820
C	-0.3710683	3.2789946	-2.0637713
C	0.4720219	2.2411011	-1.6200604
C	0.9047060	2.2497232	-0.2574209
C	1.8087565	1.2582819	0.2429621
C	2.3714828	0.2834322	-0.6769688
C	3.3660780	-0.6412432	-0.2916822
C	3.9139402	-1.5473227	-1.1867597
C	3.4641412	-1.6038648	-2.5116442
C	2.4261408	-0.7341309	-2.9304293
C	1.8936123	-0.8466838	-4.2369711
C	0.8758552	0.0170392	-4.6485162
C	0.4127211	1.0173436	-3.8072415
C	0.9169059	1.1733506	-2.4999941
C	1.9024514	0.2497225	-2.0288359
H	2.7837429	0.5098911	2.0286869
H	1.8350614	2.2177857	3.5399133
C	0.1951854	4.2077609	2.9352526
C	-0.9500514	5.3246061	1.0306653
H	-1.4504899	5.0705455	-1.5940178
H	-0.6968989	3.3081450	-3.1012853
H	3.7316744	-0.6493558	0.7326572
H	4.6817585	-2.2457832	-0.8586669
C	4.0684509	-2.5377919	-3.4603724
C	2.3637144	-1.8888649	-5.1508316
H	0.4645738	-0.1126438	-5.6495931
H	-0.3755784	1.6750029	-4.1662858
N	-0.6396216	5.2010708	2.3887479
C	-1.3109624	6.1489040	3.2997480
O	-1.6457290	6.2770169	0.6524168
O	0.3980967	4.1768987	4.1447908
N	3.4538977	-2.6619913	-4.7137940
O	5.0756893	-3.2126250	-3.2177681
O	1.8595418	-2.1049156	-6.2482162

C	3.9957529	-3.7082793	-5.6034210
C	4.0643421	-3.2494689	-7.0528604
C	-2.6979515	5.6377610	3.7508748
C	-3.5490449	6.7887265	4.2997919
H	-3.1779345	5.2905684	2.8241499
O	4.5929722	-2.0089603	-7.1467785
O	3.8207558	-3.9274084	-8.0212878
H	4.5951906	-1.7939236	-8.0969959
C	3.3456655	-5.0877131	-5.3573169
C	4.2431999	-6.2119628	-5.8871745
C	1.9114218	-5.2151551	-5.8798339
C	-0.3824711	6.6372946	4.4022841
H	5.0472277	-3.7948913	-5.2950844
H	3.3249318	-5.1930657	-4.2619180
C	-2.6506432	4.4559815	4.7229375
H	-1.4862713	7.0360327	2.6750498
H	5.6398477	-4.1871933	-1.9053356
O	0.8154281	7.0104323	3.8980902
O	-0.6853843	6.8154571	5.5570396
H	1.3451864	7.2975044	4.6635985
H	-7.7714080	4.8008877	-2.0280222
H	-7.6838718	5.5909962	-0.4309478
H	-8.8556073	4.2767704	-0.7192300
H	6.2867137	-8.4521374	-0.0493412
H	5.4118227	-9.5276052	1.0730238
H	6.0617266	-7.9777390	1.6554052
H	4.1742102	-8.4214766	-1.6657281
H	2.5796890	-8.1335563	-0.9495552
H	3.4870898	-9.5998753	-0.5065175
H	-6.2599594	2.5136590	1.3519373
H	-7.9506494	3.0548322	1.2834041
H	-6.6384159	4.2296372	1.6012725
H	-3.6296781	7.6062830	3.5658184
H	-3.1239706	7.1905340	5.2302119
H	-4.5698146	6.4334719	4.5067194
H	4.3489093	-6.1562433	-6.9799984
H	3.8100852	-7.1898351	-5.6282719
H	5.2435834	-6.1663264	-5.4284383
H	1.8841496	-5.1489783	-6.9755822
H	1.2610253	-4.4214047	-5.4898991
H	1.4932041	-6.1862122	-5.5712527
H	-2.0927154	3.6076329	4.3061469
H	-3.6755015	4.1133893	4.9336835
H	-2.1664113	4.7392598	5.6672393

PDI-valine dimer - cation (B3LYP+D3, DZP, grid 3, gas phase)

140
Energy = -4043.0058250270
C -1.5158068 0.5208415 1.9381756
C -2.4500214 1.5418474 1.7697992
C -3.0311533 1.7590607 0.5273131
C -2.7170618 0.9093963 -0.5553539
C -3.3408509 1.1267509 -1.8040243
C -3.0480374 0.2947785 -2.8770418
C -2.1236358 -0.7389387 -2.7315110
C -1.4591707 -0.9751850 -1.5153611
C -1.7667012 -0.1419348 -0.3954368
C -1.1349926 -0.3165949 0.8751376
C -0.0926243 -1.3261851 1.0065910
C 0.6281188 -1.5091836 2.1996892
C 1.6661743 -2.4349361 2.2985137
C 2.0150330 -3.2136649 1.2025357
C 1.2986803 -3.0842181 -0.0081659
C 1.6592724 -3.8897371 -1.1099169
C 0.9471211 -3.7966724 -2.2986870
C -0.0874274 -2.8709453 -2.4258505
C -0.4465838 -2.0129982 -1.3716758
C 0.2383891 -2.1371871 -0.1229177
H -1.0722928 0.3961262 2.9234048
H -2.7171397 2.1958287 2.5988459
C -3.9646614 2.9047330 0.3542290
C -4.3144793 2.2391412 -1.9988272
H -3.5513653 0.4706275 -3.8275707
H -1.9153847 -1.3641130 -3.5967168
H 0.3899793 -0.9125852 3.0773002
H 2.2215000 -2.5613260 3.2277065
C 3.1486112 -4.1737677 1.3316052
C 2.8110486 -4.8281132 -1.0266346
H 1.2267455 -4.4384379 -3.1331186
H -0.6074956 -2.8187953 -3.3796405
N -4.5781347 3.0562876 -0.8907847
C -5.5257140 4.1853096 -1.0972301
O -4.8419882 2.4303755 -3.0770484
O -4.1692923 3.6878903 1.2627584
N 3.4684013 -4.9374330 0.2003970
O 3.7714693 -4.2742172 2.3705740
O 3.1736226 -5.4617037 -2.0001588
C 4.6210657 -5.8711033 0.3223709
C 5.5418451 -5.7259951 -0.8907560
C -6.9757961 3.8395812 -0.6982450
C -7.9387365 4.9007245 -1.2482145
H -7.1882364 2.8957237 -1.2305419
O 5.8000454 -4.4169300 -1.1056417
O 6.0321296 -6.6201120 -1.5237087

C	4.1996259	-7.3070583	0.6991764
C	5.4270032	-8.1159275	1.1406912
C	3.3975491	-8.0429880	-0.3785090
C	-4.9427335	5.4706377	-0.5071005
H	5.1950008	-5.4678752	1.1675297
H	3.5542406	-7.1788956	1.5859516
C	-7.1904305	3.6067250	0.8004482
H	-5.5151932	4.3388556	-2.1846769
O	-3.6682820	5.6216551	-0.9305547
O	-5.5264119	6.2735185	0.1676026
H	-3.2422093	6.3235659	-0.3994210
C	2.4416226	1.1130625	1.4758755
C	1.8401703	1.9627582	2.4039465
C	0.8826906	2.8811142	1.9932234
C	0.5155248	2.9575932	0.6317238
C	-0.4232845	3.9315859	0.2226248
C	-0.8494965	3.9647738	-1.1007778
C	-0.3726370	3.0222680	-2.0130782
C	0.5741813	2.0491100	-1.6518541
C	1.0640497	2.0373288	-0.3095585
C	2.0705496	1.1177699	0.1206233
C	2.6566226	0.2014696	-0.8505314
C	3.7247499	-0.6565335	-0.5393807
C	4.2420970	-1.5606291	-1.4683853
C	3.6713269	-1.6649022	-2.7324202
C	2.5853963	-0.8302419	-3.0809874
C	1.9623130	-0.9958382	-4.3374642
C	0.9264556	-0.1518153	-4.7160981
C	0.4958617	0.8596666	-3.8580141
C	1.0496268	1.0278236	-2.5775669
C	2.0970864	0.1471217	-2.1643236
H	3.1975218	0.4164737	1.8313402
H	2.1057351	1.9226198	3.4602053
C	0.2242931	3.7432397	3.0130478
C	-0.9326125	4.9439150	1.1914666
H	-1.5886792	4.7048912	-1.4032961
H	-0.7517188	3.0649542	-3.0319657
H	4.1814956	-0.6257154	0.4476104
H	5.0649951	-2.2212538	-1.1998278
C	4.2283490	-2.6326752	-3.7206607
C	2.3668735	-2.0978923	-5.2529441
H	0.4617353	-0.3004607	-5.6906378
H	-0.3085551	1.5102845	-4.1935684
N	-0.6335054	4.7409793	2.5439366
C	-1.2733731	5.6703319	3.5130339
O	-1.5941316	5.8994491	0.8284478
O	0.4233937	3.5755171	4.2005863
N	3.4921819	-2.8429732	-4.8930048
O	5.2691122	-3.2297058	-3.5140871
O	1.7350805	-2.3390157	-6.2632771

C	3.9726963	-3.9225066	-5.7963528
C	3.9256189	-3.4928453	-7.2616238
C	-2.6455718	5.1568880	4.0023674
C	-3.4617000	6.3035407	4.6125225
H	-3.1658749	4.8424811	3.0843675
O	4.4024286	-2.2391117	-7.4078304
O	3.6118313	-4.1992408	-8.1821313
H	4.3784994	-2.0413879	-8.3631555
C	3.3421128	-5.2926118	-5.4623305
C	4.1672130	-6.4284567	-6.0807008
C	1.8591903	-5.4139978	-5.8274820
C	-0.2921814	6.1201720	4.5939459
H	5.0446202	-3.9950051	-5.5675048
H	3.4384399	-5.3813669	-4.3689639
C	-2.5710725	3.9553633	4.9497166
H	-1.4596954	6.5760250	2.9200033
H	6.2159187	-4.3194409	-1.9852829
O	0.9041239	6.4334790	4.0540686
O	-0.5641811	6.2816243	5.7535999
H	1.4678952	6.7448526	4.7872290
H	-7.7955799	5.0552841	-2.3292617
H	-7.7978088	5.8626201	-0.7379491
H	-8.9780374	4.5775589	-1.0933400
H	6.1004730	-8.3034383	0.2940920
H	5.1078232	-9.0856978	1.5484375
H	5.9934667	-7.5938705	1.9278436
H	3.9718596	-8.1190693	-1.3106095
H	2.4462202	-7.5410910	-0.6029084
H	3.1597743	-9.0584576	-0.0291515
H	-6.6050084	2.7562478	1.1762482
H	-8.2512048	3.3852254	0.9887605
H	-6.9105761	4.4963479	1.3789969
H	-3.5514493	7.1472146	3.9107005
H	-3.0046840	6.6676355	5.5420708
H	-4.4794468	5.9548937	4.8395143
H	4.1135785	-6.4088090	-7.1771581
H	3.7839115	-7.3981591	-5.7319035
H	5.2242004	-6.3642598	-5.7789295
H	1.7090905	-5.3120397	-6.9100749
H	1.2438503	-4.6451772	-5.3383878
H	1.4823543	-6.3981917	-5.5120300
H	-2.0450245	3.1009113	4.5002667
H	-3.5887580	3.6268374	5.2075704
H	-2.0414094	4.2143655	5.8756409

PDI-valine trimer - neutral (B3LYP+D3, DZP, grid 3, gas phase)

210
Energy = -6064.9404960830

C	-1.1640062	0.7005122	2.1095536
C	-2.0498440	1.7821842	2.0576248
C	-2.8573973	1.9707728	0.9495575
C	-2.7884305	1.0670993	-0.1352599
C	-3.6422491	1.2504390	-1.2473750
C	-3.5360182	0.4043289	-2.3389706
C	-2.5717680	-0.6088504	-2.3568851
C	-1.7109199	-0.8258795	-1.2787694
C	-1.8408479	0.0008771	-0.1194698
C	-1.0304417	-0.1915961	1.0445241
C	-0.0656606	-1.2977522	1.0614789
C	0.7006017	-1.6060215	2.1876606
C	1.6579147	-2.6260834	2.1726742
C	1.8948952	-3.3472982	1.0139714
C	1.1423768	-3.0661766	-0.1497265
C	1.4299414	-3.7602918	-1.3469556
C	0.6796285	-3.5167795	-2.4840876
C	-0.3640604	-2.5859013	-2.4546003
C	-0.6561526	-1.8459084	-1.3079083
C	0.1244485	-2.0669706	-0.1288262
H	-0.5452753	0.5914415	2.9972047
H	-2.1051632	2.4997189	2.8760263
C	-3.7386403	3.1573627	0.8832273
C	-4.6523546	2.3366605	-1.2677477
H	-4.2101731	0.5528350	-3.1822909
H	-2.5058650	-1.2367018	-3.2430938
H	0.5621652	-1.0481327	3.1115486
H	2.2388076	-2.8636420	3.0636928
C	2.9374290	-4.4029432	1.0163643
C	2.5710561	-4.6990290	-1.4150145
H	0.9288816	-4.0488872	-3.4018746
H	-0.9259553	-2.4221910	-3.3711248
N	-4.6536846	3.2211691	-0.1722732
C	-5.5858140	4.3727634	-0.2396382
O	-5.4355985	2.4726766	-2.1902575
O	-3.6716088	4.0517907	1.7111178
N	3.1951202	-5.0418483	-0.2117171
O	3.5547166	-4.6987306	2.0234844
O	2.9603092	-5.1571589	-2.4773129
C	4.3059329	-6.0243713	-0.2391414
C	5.2819570	-5.6653018	-1.3609379
C	-6.8710600	4.1796530	0.5907400
C	-7.9099129	5.2380006	0.1941553
O	5.6046958	-4.3622960	-1.2600047
O	5.7542871	-6.4206451	-2.1705149
C	3.8360489	-7.4921061	-0.1753453

C	5.0288718	-8.4074246	0.1343780
C	3.0630742	-7.9832573	-1.4035069
C	-4.8124652	5.6733616	-0.0152394
H	4.8517550	-5.8207816	0.6918254
C	-6.6677329	4.1419328	2.1087045
H	-5.8867159	4.3973581	-1.2955970
O	-3.7382689	5.6888038	-0.8265353
O	-5.1290635	6.5813645	0.7088335
H	-3.0921702	6.3568164	-0.5074132
C	2.3991985	1.4356086	1.3576447
C	1.9224239	2.4621157	2.1768004
C	1.0048655	3.3784604	1.6889883
C	0.5052426	3.2438759	0.3755227
C	-0.4266456	4.1890504	-0.1156033
C	-0.9826568	4.0092944	-1.3724761
C	-0.5960506	2.9242212	-2.1666373
C	0.3853498	2.0214153	-1.7565330
C	0.9488054	2.1690490	-0.4508499
C	1.9535618	1.2798936	0.0438924
C	2.5150644	0.2702173	-0.8599421
C	3.5780656	-0.5544764	-0.4913421
C	4.1886326	-1.4258506	-1.3998425
C	3.7115146	-1.5306903	-2.6969236
C	2.5759271	-0.7799598	-3.0843027
C	2.0352863	-0.9543214	-4.3767418
C	0.9264083	-0.2208275	-4.7665692
C	0.3721756	0.7320908	-3.9079905
C	0.8908356	0.9581946	-2.6317863
C	1.9853986	0.1547244	-2.1829494
H	3.1463064	0.7598455	1.7674500
H	2.2838049	2.5718272	3.1977004
C	0.5609729	4.4892656	2.5581862
C	-0.7733475	5.3850610	0.6864861
H	-1.7354925	4.7102516	-1.7275445
H	-1.0577796	2.8225774	-3.1456543
H	3.9855572	-0.5048194	0.5153596
H	5.0309652	-2.0409664	-1.0899681
C	4.4114381	-2.3904903	-3.6789061
C	2.6362689	-1.9162097	-5.3257506
H	0.5125759	-0.3810596	-5.7606376
H	-0.4751247	1.3120676	-4.2664901
N	-0.3467123	5.4088565	2.0149388
C	-0.7733446	6.5676671	2.8417343
O	-1.3910465	6.3312307	0.2118923
O	0.9779492	4.6220984	3.6963989
N	3.7749041	-2.6140051	-4.9003348
O	5.5130418	-2.8773405	-3.4510916
O	2.1799621	-2.0886592	-6.4433331
C	4.4303104	-3.5607455	-5.8400214
C	4.5312836	-2.9269454	-7.2272713

C	-2.0071216	6.2642055	3.7146818
C	-2.6010158	7.5740789	4.2488673
O	5.0471388	-1.6874842	-7.1005810
O	4.2764060	-3.4529367	-8.2779736
H	4.8868144	-1.1625534	-7.9109690
C	3.8518340	-4.9869387	-5.7531950
C	4.7903242	-5.9744331	-6.4584301
C	2.4107988	-5.1240495	-6.2517889
C	0.4441536	7.1810054	3.5332418
H	5.4654980	-3.6083372	-5.4779788
C	-1.7636886	5.2565185	4.8413744
H	-1.0792760	7.3153372	2.0985563
H	5.9897935	-4.0500681	-2.1086176
O	1.4177030	7.3570681	2.6169345
O	0.5195038	7.5294698	4.6815137
H	2.2821314	7.4991067	3.0532139
H	2.5346866	6.7450938	0.6318813
O	3.9627780	6.4919402	2.7294087
H	1.8401433	6.1854517	-1.6582933
C	2.9905770	5.9000289	0.1184284
H	5.1935141	5.8482069	4.4090936
C	2.6022485	5.5689977	-1.1859985
C	4.3003210	5.4518364	2.1828817
H	1.0691814	5.4741493	-3.3488360
C	3.9150464	5.1165458	0.7914074
C	5.2653419	4.7551845	4.3240784
C	1.6264341	4.6856925	-3.8498704
H	0.2919814	4.6917367	-5.5616573
C	4.0990185	4.8256213	6.5702951
C	4.1330052	4.1585740	5.1900004
N	5.0593917	4.5001940	2.8794337
O	7.5880640	4.9334759	3.8906478
C	6.6894184	4.4356216	4.7656120
C	1.1796449	4.2562367	-5.1031268
C	3.1551669	4.4848474	-1.8708777
C	2.7191665	4.0902909	-3.2173858
O	6.9984906	3.9188029	5.8086778
C	4.4891337	3.9970441	0.1402285
H	8.4681205	4.7058238	4.2434882
C	4.1578089	3.7017297	-1.2168282
C	4.1639244	2.6311464	5.3070878
O	0.2517087	3.1555090	-7.5227483
C	5.6105222	3.3501248	2.2985160
C	1.8539957	3.2554151	-5.7839365
C	5.3737995	3.1533457	0.8504219
C	1.3197837	2.7726634	-7.0775131
C	3.4141127	3.0380008	-3.8939898
O	6.2417413	2.5509427	2.9682129
C	-0.6320108	0.2561772	-8.2848994
C	3.0038220	2.6659853	-5.2102100

C	4.8204550	2.6185207	-1.8768097
O	0.0152767	2.2718061	-10.6274493
C	4.4949433	2.3301916	-3.2800476
C	5.9852438	2.0928359	0.2015886
C	0.7572117	0.0194183	-8.8865385
C	0.9951874	2.3926865	-9.9376496
N	2.0924277	1.8308027	-7.7700685
H	1.3383301	4.1345890	-10.5353572
C	5.7327789	1.8499629	-1.1519405
O	1.7790846	3.4909985	-9.9502772
C	1.6029982	1.3007208	-9.0638402
C	3.7250351	1.6864041	-5.9363608
C	0.6706654	-0.7587513	-10.2050587
H	6.6576204	1.4512777	0.7709023
C	3.3218346	1.3298199	-7.3174611
C	5.1705738	1.3635028	-4.0273912
C	4.8104443	1.0582512	-5.3458633
H	6.2342631	1.0083348	-1.6245754
H	2.5215019	1.0096544	-9.5917482
H	5.9999933	0.8120544	-3.5892573
O	3.9980970	0.6110439	-8.0387883
H	5.3471994	0.2895094	-5.8989314
H	4.6788738	-9.4334401	0.3206421
H	5.5734072	-8.0721597	1.0313858
H	5.7321399	-8.4308512	-0.7090018
H	2.7910796	-9.0411705	-1.2671837
H	3.6739186	-7.8900331	-2.3103617
H	2.1342837	-7.4190522	-1.5603148
H	4.8224295	-5.7891078	-7.5408866
H	4.4414695	-7.0041444	-6.2925162
H	5.8143785	-5.9063120	-6.0587218
H	2.3261747	-4.8270683	-7.3053988
H	1.7157333	-4.5025877	-5.6704934
H	2.0851435	-6.1700971	-6.1486548
H	-1.2535382	0.8619975	-8.9570010
H	-0.5835895	0.7837412	-7.3226454
H	-1.1300966	-0.7113683	-8.1190244
H	0.1071436	-0.1963143	-10.9618441
H	0.1645824	-1.7209276	-10.0382554
H	1.6731956	-0.9794795	-10.6035670
H	-8.0781885	5.2509439	-0.8944519
H	-7.5849817	6.2397533	0.5062500
H	-8.8735151	5.0211963	0.6782297
H	-6.2043793	5.0717258	2.4622918
H	-6.0287569	3.3048786	2.4194296
H	-7.6419008	4.0202938	2.6066506
H	-2.8207791	8.2764148	3.4294079
H	-1.9156717	8.0621630	4.9553898
H	-3.5483728	7.3699896	4.7688909
H	-1.4508421	4.2768987	4.4545196

H	-2.6956852	5.1073092	5.4071919
H	-0.9835421	5.6110885	5.5277056
H	4.0131560	5.9198619	6.4813884
H	5.0029720	4.5890021	7.1478992
H	3.2233036	4.4725312	7.1343650
H	4.1627061	2.1398969	4.3246650
H	3.2779537	2.2874845	5.8627487
H	5.0646114	2.2954577	5.8372832
H	3.2047210	4.4474162	4.6712657
H	1.3374035	-0.6011660	-8.1846663
H	-2.7395291	5.8266292	3.0191549
H	3.8638578	-5.2278252	-4.6794031
H	-7.2604899	3.1974982	0.2694703
H	3.1583738	-7.5259659	0.6959295

PDI-valine trimer - anion (B3LYP+D3, DZP, grid 3, gas phase)

210
Energy = -6065.0636604700
C -1.1218410 0.7143368 2.0998993
C -2.0260352 1.7808661 2.0680675
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C -0.0478004 -1.2932068 1.0456386
C 0.7162887 -1.6124770 2.1701156
C 1.6500970 -2.6532715 2.1554023
C 1.8679972 -3.3847265 0.9993964
C 1.1253434 -3.0849828 -0.1661907
C 1.3983689 -3.7835018 -1.3643560
C 0.6697148 -3.5049676 -2.5078013
C -0.3521053 -2.5507533 -2.4788505
C -0.6450355 -1.8241278 -1.3242490
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H -2.0701915 2.5000922 2.8853231
C -3.7843557 3.1103112 0.9483266
C -4.6904218 2.3080851 -1.2150085
H -4.2284942 0.5606227 -3.1560551
H -2.4944022 -1.1997187 -3.2509487
H 0.5951155 -1.0446683 3.0901531
H 2.2307777 -2.8983184 3.0443806
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C 5.2050345 -5.7066908 -1.3927550
C -6.9121162 4.1706394 0.6382611
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O 5.4995482 -4.4066463 -1.2892860
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C 3.7941150 -7.5573456 -0.1884996

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C	-4.8146650	5.6287761	0.0531370
H	4.7945152	-5.8741211	0.6667128
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H	-5.9078711	4.3719646	-1.2363326
O	-3.7413317	5.6136939	-0.7439022
O	-5.1298592	6.5401634	0.7785540
H	-3.0039960	6.1741396	-0.3794468
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C	1.9744029	2.4445333	2.1716783
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C	0.5225946	3.2418261	0.3858999
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C	-0.5959348	2.9353713	-2.1643170
C	0.3976262	2.0161863	-1.7551146
C	0.9625141	2.1624614	-0.4498797
C	1.9706209	1.2685219	0.0325833
C	2.5157947	0.2718469	-0.8637598
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C	4.1882872	-1.4297478	-1.3983041
C	3.7044648	-1.5391724	-2.7115204
C	2.5719026	-0.7805372	-3.0980844
C	2.0324352	-0.9317271	-4.3954712
C	0.9121425	-0.1815729	-4.7769452
C	0.3610536	0.7498543	-3.9178395
C	0.8913400	0.9706137	-2.6251085
C	1.9838236	0.1571104	-2.1859874
H	3.1722817	0.7354350	1.7620786
H	2.3446846	2.5597255	3.1889229
C	0.6363914	4.4860382	2.5462727
C	-0.7806213	5.3464199	0.7056501
H	-1.7278322	4.7055620	-1.7264195
H	-1.0554356	2.8336181	-3.1443259
H	3.9998639	-0.5170275	0.5093135
H	5.0285570	-2.0483241	-1.0915160
C	4.3717291	-2.4115722	-3.6719485
C	2.6350230	-1.8558353	-5.3496318
H	0.5030145	-0.3337010	-5.7743421
H	-0.4912243	1.3313291	-4.2613323
N	-0.3099179	5.3829904	2.0204105
C	-0.7559055	6.5146018	2.8639364
O	-1.4669226	6.2870636	0.2780889
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N	3.7501773	-2.5903954	-4.9101809
O	5.4506061	-2.9800278	-3.4446873
O	2.2212397	-2.0024181	-6.4979181
C	4.3789666	-3.5508240	-5.8446095
C	4.5336522	-2.9140205	-7.2227052

C	-1.9515113	6.1567826	3.7692549
C	-2.5949330	7.4381627	4.3145289
O	5.1218447	-1.7085276	-7.0790614
O	4.2759137	-3.4177689	-8.2865034
H	4.9436907	-1.1416811	-7.8573368
C	3.7403203	-4.9527654	-5.7821200
C	4.6572896	-5.9767148	-6.4628511
C	2.3098938	-5.0321111	-6.3231584
C	0.4499695	7.1758566	3.5253064
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C	-1.6359783	5.1658047	4.8934863
H	-1.1163344	7.2519605	2.1345256
H	5.7679510	-4.0191718	-2.1658750
O	1.3777986	7.4251907	2.5784620
O	0.5485372	7.5187033	4.6762311
H	2.2634525	7.5359048	2.9806677
H	2.4342185	6.7517601	0.5951702
O	3.9136936	6.5864786	2.6850425
H	1.7566148	6.1451156	-1.6846972
C	2.9156205	5.9148865	0.0919170
H	5.1144208	5.9814166	4.3710990
C	2.5373619	5.5578119	-1.2068491
C	4.2468568	5.5337012	2.1552452
H	1.0558753	5.4470177	-3.3958253
C	3.8592310	5.1635701	0.7769437
C	5.2331709	4.8910059	4.3025648
C	1.6293872	4.6644887	-3.8868134
H	0.3328262	4.6643678	-5.6241683
C	4.0847141	4.9630341	6.5562299
C	4.1376429	4.2627054	5.1931094
N	5.0232086	4.6068577	2.8669883
O	7.5430924	5.1572029	3.8314363
C	6.6735903	4.6435579	4.7298531
C	1.2116990	4.2322355	-5.1464653
C	3.1203024	4.4798802	-1.8793188
C	2.7110947	4.0738332	-3.2290230
O	7.0255066	4.1718341	5.7823419
C	4.4534472	4.0421148	0.1453082
H	8.4321955	4.9597443	4.1782522
C	4.1297421	3.7202677	-1.2082449
C	4.2388560	2.7419090	5.3468372
O	0.3549335	3.1466710	-7.6054363
C	5.6018948	3.4607300	2.3044927
C	1.8980208	3.2252088	-5.8081809
C	5.3538474	3.2260529	0.8676690
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C	3.4187201	3.0173781	-3.8855149
O	6.2755273	2.7063537	2.9882883
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C	3.0320202	2.6335783	-5.2061014

C	4.8044642	2.6326957	-1.8480094
O	0.2265474	2.2611690	-10.7204922
C	4.4881483	2.3157742	-3.2452985
C	5.9778375	2.1602714	0.2372768
C	0.8368321	0.0036239	-8.9243355
C	1.1750408	2.3609740	-9.9825357
N	2.1791286	1.7909935	-7.7774283
H	1.5661145	4.0929396	-10.5691629
C	5.7231868	1.8853809	-1.1070531
O	1.9813802	3.4456987	-9.9704965
C	1.7197139	1.2625843	-9.0794272
C	3.7652384	1.6441093	-5.9081827
C	0.7941575	-0.7893572	-10.2361916
H	6.6564594	1.5364257	0.8182712
C	3.3971603	1.2884585	-7.2953040
C	5.1664030	1.3285034	-3.9655779
C	4.8307589	1.0106831	-5.2856880
H	6.2225014	1.0326051	-1.5606376
H	2.6486356	0.9428541	-9.5720405
H	5.9755925	0.7692480	-3.5015448
O	4.0924423	0.5797347	-8.0124057
H	5.3664115	0.2247514	-5.8151036
H	4.6739462	-9.4875066	0.2990193
H	5.5447901	-8.1100747	1.0114810
H	5.7033949	-8.4574942	-0.7309418
H	2.7706624	-9.1297231	-1.2707091
H	3.6291719	-7.9619115	-2.3200790
H	2.0870169	-7.5160086	-1.5655726
H	4.7411620	-5.7781242	-7.5407450
H	4.2549859	-6.9918899	-6.3263914
H	5.6662040	-5.9610239	-6.0209664
H	2.2705328	-4.7337497	-7.3790879
H	1.6268633	-4.3756660	-5.7677128
H	1.9371684	-6.0639787	-6.2262532
H	-1.1484456	0.8955997	-9.0900208
H	-0.5518058	0.8050379	-7.4260568
H	-1.0992153	-0.6772728	-8.2409060
H	0.2854483	-0.2226966	-11.0286976
H	0.2539099	-1.7353294	-10.0826179
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H	-7.5802508	6.2425179	0.5344029
H	-8.8998955	5.0549544	0.7065030
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H	-6.1062146	3.2919168	2.4793984
H	-7.7120462	4.0352320	2.6463904
H	-2.8812130	8.1176971	3.4961956
H	-1.9087828	7.9689359	4.9896725
H	-3.5108753	7.1920039	4.8726804
H	-1.2764880	4.2048798	4.5018661

H	-2.5489478	4.9705900	5.4779143
H	-0.8599745	5.5619258	5.5615773
H	3.9374732	6.0483338	6.4392368
H	5.0065082	4.7906924	7.1294669
H	3.2346549	4.5794623	7.1398249
H	4.2370269	2.2288373	4.3766161
H	3.3774486	2.3752551	5.9263053
H	5.1627317	2.4574677	5.8678309
H	3.1933412	4.4937184	4.6759094
H	1.3694327	-0.6193156	-8.1888092
H	-2.6798365	5.6832223	3.0932725
H	3.7111711	-5.1977567	-4.7094706
H	-7.3159171	3.1942846	0.3163241
H	3.1217761	-7.6004991	0.6867644

PDI-valine trimer - cation (B3LYP+D3, DZP, grid 3, gas phase)

210
Energy = -6064.6804752810
C -1.2227532 0.7592466 2.0663819
C -2.1107678 1.8327370 1.9683581
C -2.8445266 2.0276454 0.8085010
C -2.7196527 1.1181688 -0.2650181
C -3.5066831 1.3066924 -1.4237759
C -3.3654412 0.4426613 -2.5000416
C -2.4273889 -0.5911235 -2.4539688
C -1.6183482 -0.8073646 -1.3304186
C -1.7842022 0.0435810 -0.1929985
C -1.0192810 -0.1299811 1.0031456
C -0.0173371 -1.1945623 1.0517064
C 0.7720027 -1.4300146 2.1854108
C 1.7763635 -2.4007018 2.1970116
C 2.0335389 -3.1540558 1.0607216
C 1.2532420 -2.9586830 -0.1015890
C 1.5503136 -3.7034258 -1.2643095
C 0.7690878 -3.5533964 -2.3996412
C -0.2905591 -2.6438900 -2.4085598
C -0.5812318 -1.8382516 -1.3000418
C 0.2012378 -1.9952219 -0.1130122
H -0.6619370 0.6465683 2.9912460
H -2.2223290 2.5436056 2.7870051
C -3.7157780 3.2236377 0.6909222
C -4.4979729 2.4133514 -1.5100786
H -3.9948977 0.5928448 -3.3770683
H -2.3354726 -1.2355823 -3.3254756
H 0.6140664 -0.8488020 3.0912672
H 2.3760263 -2.5792427 3.0894898
C 3.1251079 -4.1652211 1.0944623
C 2.7255437 -4.6090513 -1.3047207
H 1.0126177 -4.1378300 -3.2868167
H -0.8739331 -2.5525155 -3.3217115
N -4.5607532 3.2968916 -0.4185904
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O -5.2080229 2.5549875 -2.4867278
O -3.6846396 4.1116984 1.5253802
N 3.3869312 -4.8581940 -0.1003012
O 3.7706369 -4.3695066 2.1041845
O 3.1041672 -5.1052502 -2.3518182
C 4.5106059 -5.8309289 -0.0827633
C 5.4531342 -5.5567678 -1.2543758
C -6.8421734 4.1883104 0.2177918
C -7.8793961 5.2361831 -0.2093298
O 5.7748869 -4.2437162 -1.2707428
O 5.9107988 -6.3670754 -2.0135462
C 4.0500005 -7.2916476 0.1043339

C	5.2551927	-8.1799791	0.4427916
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C	-4.7898662	5.7452289	-0.2201583
H	5.0805772	-5.5528791	0.8137347
C	-6.7253270	4.1046990	1.7428839
H	-5.7438002	4.4778585	-1.5979838
O	-3.6582801	5.8124433	-0.9570140
O	-5.1742829	6.6275733	0.4982670
H	-3.1029532	6.5387601	-0.6079210
C	2.4446185	1.4220340	1.3323248
C	1.9563584	2.4205991	2.1741147
C	1.0376418	3.3479795	1.7000278
C	0.5483603	3.2462117	0.3814396
C	-0.3781161	4.2040827	-0.0894514
C	-0.9319769	4.0641868	-1.3553463
C	-0.5498741	2.9982523	-2.1713483
C	0.4262687	2.0717479	-1.7735160
C	0.9927459	2.1919775	-0.4678774
C	1.9996624	1.2953511	0.0079213
C	2.5518655	0.3090718	-0.9115969
C	3.6308270	-0.5189683	-0.5660975
C	4.2104211	-1.3968792	-1.4831514
C	3.6897577	-1.5056235	-2.7659385
C	2.5519332	-0.7496680	-3.1288983
C	1.9775024	-0.9339823	-4.4034383
C	0.8647174	-0.1919495	-4.7776842
C	0.3477325	0.7798598	-3.9214890
C	0.9001687	1.0103549	-2.6527549
C	1.9934554	0.1961773	-2.2213485
H	3.1896955	0.7364709	1.7288627
H	2.3061767	2.5037551	3.2015388
C	0.5739987	4.4335114	2.6027548
C	-0.7275853	5.3870108	0.7426689
H	-1.6833007	4.7784072	-1.6884802
H	-1.0104038	2.9176107	-3.1527707
H	4.0613335	-0.4666045	0.4307307
H	5.0546790	-2.0221111	-1.1972568
C	4.3608693	-2.3831867	-3.7622870
C	2.5398891	-1.9267852	-5.3557256
H	0.4226952	-0.3635107	-5.7576282
H	-0.5023319	1.3650108	-4.2642289
N	-0.3276934	5.3659003	2.0795182
C	-0.7720176	6.4991914	2.9368802
O	-1.3207806	6.3428741	0.2707031
O	0.9813343	4.5175131	3.7462625
N	3.6771575	-2.6342102	-4.9524876
O	5.4697554	-2.8478285	-3.5551051
O	2.0400454	-2.1010822	-6.4512545
C	4.2946768	-3.6079120	-5.8945895
C	4.3834788	-2.9897675	-7.2900230

C	-2.0096364	6.1582427	3.7915007
C	-2.6135275	7.4462129	4.3673629
O	4.9112379	-1.7504289	-7.1857373
O	4.1053298	-3.5228615	-8.3287719
H	4.8027196	-1.2742869	-8.0319759
C	3.6855783	-5.0200855	-5.7806619
C	4.5831634	-6.0330909	-6.5038939
C	2.2294504	-5.1293917	-6.2419097
C	0.4349455	7.1032590	3.6550609
H	5.3354317	-3.6740283	-5.5523719
C	-1.7669395	5.1144830	4.8853336
H	-1.0783690	7.2654923	2.2132804
H	6.1979628	-4.0388302	-2.1291998
O	1.4253867	7.2982701	2.7569590
O	0.4935615	7.4265457	4.8094432
H	2.2566679	7.5093936	3.2249097
H	2.5637624	6.6615026	0.7412345
O	3.9689608	6.3252296	2.8188052
H	1.8734141	6.1856979	-1.5731031
C	3.0119742	5.8309332	0.1963018
H	5.2309789	5.6374283	4.4875971
C	2.6264084	5.5464878	-1.1168810
C	4.3161755	5.3043829	2.2522271
H	1.1124274	5.5458990	-3.2931462
C	3.9311818	5.0148816	0.8435928
C	5.2865233	4.5462106	4.3745701
C	1.6334470	4.7355497	-3.7979026
H	0.2652407	4.7696125	-5.4811593
C	4.1366848	4.5661914	6.6295833
C	4.1502306	3.9413467	5.2290395
N	5.0712302	4.3305071	2.9206769
O	7.6072809	4.6945405	3.9263257
C	6.7104537	4.1931672	4.7989352
C	1.1495478	4.3130842	-5.0368937
C	3.1744590	4.4744598	-1.8375071
C	2.7262926	4.1100194	-3.1802527
O	7.0112711	3.6420325	5.8246772
C	4.5053583	3.9213297	0.1545940
H	8.4909994	4.4637359	4.2697316
C	4.1741810	3.6678918	-1.2098157
C	4.1597141	2.4104489	5.2998425
O	0.1133480	3.1935262	-7.3883242
C	5.6089315	3.1974480	2.3043105
C	1.7830228	3.2860429	-5.7218663
C	5.3852352	3.0551838	0.8415582
C	1.1964667	2.7998526	-6.9983308
C	3.3890534	3.0488954	-3.8739386
O	6.2165560	2.3544957	2.9371959
C	-0.8182928	0.3188241	-8.1928896
C	2.9368830	2.6803741	-5.1761315

C	4.8277656	2.5979241	-1.8986564
O	-0.2001147	2.3572367	-10.5204260
C	4.4737839	2.3232929	-3.2899790
C	6.0108435	2.0205371	0.1610009
C	0.5528312	0.0732875	-8.8320103
C	0.7955558	2.4611210	-9.8539039
N	1.9342274	1.8548998	-7.7163606
H	1.1579501	4.2092592	-10.4336545
C	5.7561925	1.8158623	-1.1960097
O	1.5881255	3.5515269	-9.8553146
C	1.4102035	1.3463568	-9.0100111
C	3.6127642	1.6833004	-5.9174666
C	0.4226078	-0.6806418	-10.1612851
H	6.6908948	1.3698268	0.7104753
C	3.1647690	1.3330747	-7.2936278
C	5.1145787	1.3395369	-4.0584729
C	4.7087887	1.0357560	-5.3611844
H	6.2690310	0.9975073	-1.6962841
H	2.3140889	1.0536024	-9.5612290
H	5.9513546	0.7800013	-3.6454821
O	3.8157147	0.6006243	-8.0170753
H	5.2130707	0.2581909	-5.9344254
H	4.9114801	-9.1859808	0.7229860
H	5.8302554	-7.7761967	1.2909297
H	5.9284262	-8.2745373	-0.4195932
H	2.9780896	-8.9142912	-0.8426749
H	3.8158393	-7.8367673	-1.9928331
H	2.2985028	-7.3221505	-1.2208270
H	4.5773362	-5.8659960	-7.5893643
H	4.2241939	-7.0536688	-6.3087442
H	5.6228600	-5.9756419	-6.1455455
H	2.1223863	-4.8282701	-7.2921660
H	1.5571627	-4.4996786	-5.6414199
H	1.8888824	-6.1698666	-6.1361663
H	-1.4447590	0.9488054	-8.8372995
H	-0.7417997	0.8250982	-7.2200194
H	-1.3296709	-0.6434015	-8.0385434
H	-0.1578433	-0.1009989	-10.8912183
H	-0.0865385	-1.6412438	-9.9966731
H	1.4109441	-0.9015259	-10.5931140
H	-7.9777290	5.2850693	-1.3052369
H	-7.6052270	6.2335262	0.1594863
H	-8.8652836	4.9761369	0.2018361
H	-6.3004829	5.0292971	2.1540463
H	-6.0944316	3.2650762	2.0652308
H	-7.7237191	3.9524586	2.1788790
H	-2.8179144	8.1831755	3.5750313
H	-1.9425511	7.9041886	5.1064527
H	-3.5696024	7.2204458	4.8607903
H	-1.4573179	4.1445405	4.4702251

H	-2.6976328	4.9508464	5.4482149
H	-0.9865222	5.4455042	5.5828366
H	4.0743769	5.6640702	6.5757580
H	5.0375028	4.2927665	7.1949104
H	3.2566377	4.2138005	7.1867243
H	4.1387438	1.9461605	4.3035331
H	3.2777342	2.0626293	5.8587742
H	5.0620038	2.0461877	5.8075243
H	3.2232177	4.2623746	4.7262193
H	1.1438633	-0.5672394	-8.1568832
H	-2.7347513	5.7418620	3.0742471
H	3.7226672	-5.2514937	-4.7043046
H	-7.1887320	3.2091709	-0.1571462
H	3.4011365	-7.2618728	0.9973438