SUPPORTING INFORMATION for

Molecular interactions in diffusion-controlled aldol condensation with mesoporous silica nanoparticles

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TABLE S1. Cartesian coordinates at equilibrium points for acetone dimer in four different configurations.

Acetone dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.0115662	0.11488955	-0.0037582
O	8	-0.0054936	1.3457191	0.01703516
C	6	-1.3014216	-0.6723754	-0.0343055
C	6	1.27066004	-0.685491	-0.0004346
H	1	2.12014818	-0.0177386	0.2161532
H	1	1.21336973	-1.5037359	0.74794924
H	1	1.40555763	-1.1551127	-0.9989194
H	1	-2.1444435	0.01087671	-0.2258338
H	1	-1.4399505	-1.1765671	0.94644451
H	1	-1.2524308	-1.4635377	-0.8117157
C	6	-0.0071673	-0.0513192	3.21364689
O	8	0.01652749	-1.2819822	3.1958189
C	6	1.25380027	0.76930952	3.0688169
C	6	-1.2989453	0.71548927	3.38109517
H	1	-2.1046822	0.02014104	3.6669488
H	1	-1.1787716	1.51273727	4.14453411
H	1	-1.5522186	1.21044731	2.41850328
H	1	2.08598685	0.11377595	2.76559496
H	1	1.48702097	1.24804044	4.04436541
H	1	1.10280049	1.58131373	2.32682467
Acetone dimer in linear configuration				

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.0115662	0.11488955	-0.0037582
O	8	-0.0054936	1.3457191	0.01703516
C	6	-1.3014216	-0.6723754	-0.0343055
C	6	1.27066004	-0.685491	-0.0004346
H	1	2.12014818	-0.0177386	0.2161532
H	1	1.21336973	-1.5037359	0.74794924
H	1	1.40555763	-1.1551127	-0.9989194
H	1	-2.1444435	0.01087671	-0.2258338
H	1	-1.4399505	-1.1765671	0.94644451
H	1	-1.2524308	-1.4635377	-0.8117157
C	6	-0.0115662	-4.8851104	-0.0037582
O	8	-0.0054936	-3.6542809	0.01703516
C	6	-1.3014216	-5.6723757	-0.0343055
C	6	1.27066004	-5.6854911	-0.0004346
H	1	2.12014818	-5.0177388	0.2161532
H	1	1.21336973	-6.5037355	0.74794924
H	1	1.40555763	-6.1551127	-0.9989194
H	1	-2.1444435	-4.9891233	-0.2258338
H	1	-1.4399505	-6.1765671	0.94644451
H	1	-1.2524308	-6.4635377	-0.8117157

Acetone dimer in T-shaped configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.0115662	0.11488955	-0.0037582
O	8	-0.0054936	1.3457191	0.01703516
C	6	-1.3014216	-0.6723754	-0.0343055
C	6	1.27066004	-0.685491	-0.0004346
H	1	2.12014818	-0.0177386	0.2161532
H	1	1.21336973	-1.5037359	0.74794924
H	1	1.40555763	-1.1551127	-0.9989194
H	1	-2.1444435	0.01087671	-0.2258338
H	1	-1.4399505	-1.1765671	0.94644451
H	1	-1.2524308	-1.4635377	-0.8117157
C	6	0.01575449	0.02191617	4.15645266
O	8	0.02232694	-0.0181758	2.92610312
C	6	-1.2699583	0.15591508	4.93967295
C	6	1.29315305	-0.0607883	4.96027899

H	1	2.15891576	0.0389601	4.28578806
H	1	1.31021333	0.72871464	5.7408433
H	1	1.33047795	-1.043515	5.47851515
H	1	-2.1284864	0.01440243	4.26357651
H	1	-1.3114407	1.16897178	5.39493704
H	1	-1.2961494	-0.5829559	5.76797724
Acetone dimer in parallel-displaced configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.0115662	0.11488955	-0.0037582
O	8	-0.0054936	1.3457191	0.01703516
C	6	-1.3014216	-0.6723754	-0.0343055
C	6	1.27066004	-0.685491	-0.0004346
H	1	2.12014818	-0.0177386	0.2161532
H	1	1.21336973	-1.5037359	0.74794924
H	1	1.40555763	-1.1551127	-0.9989194
H	1	-2.1444435	0.01087671	-0.2258338
H	1	-1.4399505	-1.1765671	0.94644451
H	1	-1.2524308	-1.4635377	-0.8117157
C	6	-0.0071673	0.34868082	3.21364689
O	8	0.01652749	-0.8819822	3.1958189
C	6	1.25380027	1.1693095	3.0688169
C	6	-1.2989453	1.11548924	3.38109517
H	1	-2.1046822	0.42014104	3.6669488
H	1	-1.1787716	1.91273725	4.14453411
H	1	-1.5522186	1.61044741	2.41850328
H	1	2.08598685	0.51377594	2.76559496
H	1	1.48702097	1.64804041	4.04436541
H	1	1.10280049	1.98131371	2.32682467

TABLE S2. Cartesian coordinates at equilibrium points for hexane dimer in three different configurations. (a) *trans*-Sandwich (b) T-shaped (c) Cross

Hexane dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.1916871	0.220534	-0.000079

C	6	3.191679	-0.22064	-0.000109
C	6	-0.6624965	0.37542349	0.000084
C	6	0.66248655	-0.3755329	0.0001387
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.8753073	-0.5466147	-0.0000397
H	1	4.0495882	0.45090935	-0.0003181
H	1	-4.0495982	-0.4510131	-0.0001514
H	1	-3.267195	0.85966712	-0.8804229
H	1	-3.2673273	0.8595553	0.8803367
H	1	3.26739216	-0.8596207	0.88033277
H	1	3.26711679	-0.8598127	-0.8804275
H	1	-1.8284242	-1.1999787	0.87536758
H	1	-1.8283005	-1.1998738	-0.8755182
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.8754175
H	1	-0.7073762	1.03037131	-0.8763072
H	1	-0.7075243	1.0303061	0.87652022
H	1	0.70745343	-1.0303799	0.87660414
H	1	0.70742667	-1.0305164	-0.8762234
C	6	-3.1916871	0.220534	4.09992123
C	6	3.191679	-0.22064	4.09989119
C	6	-0.6624965	0.37542349	4.1000843
C	6	0.66248655	-0.3755329	4.10013866
C	6	1.87529767	0.54650563	4.10002184
C	6	-1.8753073	-0.5466147	4.09996033
H	1	4.0495882	0.45090935	4.09968185
H	1	-4.0495982	-0.4510131	4.09984875
H	1	-3.267195	0.85966712	3.21957707
H	1	-3.2673273	0.8595553	4.98033667
H	1	3.26739216	-0.8596207	4.98033237
H	1	3.26711679	-0.8598127	3.21957254
H	1	-1.8284242	-1.1999787	4.97536755
H	1	-1.8283005	-1.1998738	3.22448182
H	1	1.82844031	1.19982517	4.97546816
H	1	1.8282634	1.19980919	3.22458243
H	1	-0.7073762	1.03037131	3.22369289
H	1	-0.7075243	1.0303061	4.97652006
H	1	0.70745343	-1.0303799	4.97660398
H	1	0.70742667	-1.0305164	3.22377658

Hexane dimer in T-shaped configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.1916871	0.220534	-0.000079
C	6	3.191679	-0.22064	-0.000109
C	6	-0.6624965	0.37542349	0.000084
C	6	0.66248655	-0.3755329	0.0001387
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.8753073	-0.5466147	-0.0000397
H	1	4.0495882	0.45090935	-0.0003181
H	1	-4.0495982	-0.4510131	-0.0001514
H	1	-3.267195	0.85966712	-0.8804229
H	1	-3.2673273	0.8595553	0.8803367
H	1	3.26739216	-0.8596207	0.88033277
H	1	3.26711679	-0.8598127	-0.8804275
H	1	-1.8284242	-1.1999787	0.87536758
H	1	-1.8283005	-1.1998738	-0.8755182
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.8754175
H	1	-0.7073762	1.03037131	-0.8763072
H	1	-0.7075243	1.0303061	0.87652022
H	1	0.70745343	-1.0303799	0.87660414
H	1	0.70742667	-1.0305164	-0.8762234
C	6	0.39806202	-0.015773	10.1685467
C	6	-0.4034346	0.00096062	3.82037139
C	6	0.40959141	-0.0024344	7.63467836
C	6	-0.4149588	-0.0127887	6.35423899
C	6	0.4367927	0.0115024	5.09130764
C	6	-0.4421647	-0.026485	8.89761066
H	1	0.21835804	0.01867334	2.9259181
H	1	-0.223734	-0.0332043	11.0630026
H	1	1.0221585	0.87740922	10.2124443
H	1	1.05835319	-0.8829549	10.2033672
H	1	-1.0273886	-0.8923154	3.77625966
H	1	-1.0638634	0.8680414	3.78576016
H	1	-1.0789487	-0.915145	8.88312149
H	1	-1.1149463	0.83534735	8.89215469
H	1	1.10962558	-0.850296	5.0966115
H	1	1.07352424	0.90019268	5.10595226

H	1	1.04782271	0.88725054	7.64708424
H	1	1.08390129	-0.8651823	7.638062
H	1	-1.0530928	-0.9025455	6.34174061
H	1	-1.0893629	0.84988266	6.35094881

Hexane dimer in cross configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.1916871	0.220534	-0.000079
C	6	3.191679	-0.22064	-0.000109
C	6	-0.6624965	0.37542349	0.000084
C	6	0.66248655	-0.3755329	0.0001387
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.8753073	-0.5466147	-0.0000397
H	1	4.0495882	0.45090935	-0.0003181
H	1	-4.0495982	-0.4510131	-0.0001514
H	1	-3.267195	0.85966712	-0.8804229
H	1	-3.2673273	0.8595553	0.8803367
H	1	3.26739216	-0.8596207	0.88033277
H	1	3.26711679	-0.8598127	-0.8804275
H	1	-1.8284242	-1.1999787	0.87536758
H	1	-1.8283005	-1.1998738	-0.8755182
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.8754175
H	1	-0.7073762	1.03037131	-0.8763072
H	1	-0.7075243	1.0303061	0.87652022
H	1	0.70745343	-1.0303799	0.87660414
H	1	0.70742667	-1.0305164	-0.8762234
C	6	0.17479113	3.19362903	3.97275496
C	6	-0.1747974	-3.1937459	3.82705784
C	6	0.36588714	0.66745222	3.92071056
C	6	-0.3659037	-0.6675761	3.87951279
C	6	0.57329899	-1.8670943	3.86852479
C	6	-0.5733112	1.86697519	3.93145776
H	1	0.50889081	-4.0419793	3.81948185
H	1	-0.5088903	4.04187059	3.98004985
H	1	0.82712716	3.29731941	3.10505462
H	1	0.7981391	3.25889015	4.86515617
H	1	-0.8269798	-3.2976413	4.69485378
H	1	-0.7983012	-3.2588093	2.9347558

H	1	-1.2402041	1.79180932	4.79460621
H	1	-1.2113848	1.83003044	3.04437447
H	1	1.21143591	-1.8302974	4.75557375
H	1	1.24012971	-1.7917774	3.00534725
H	1	1.03440821	0.74065912	3.05656195
H	1	1.00559664	0.70242029	4.80873537
H	1	-1.0343238	-0.7408704	4.74373531
H	1	-1.0057163	-0.7024596	2.99156237

TABLE S3. Cartesian coordinates at equilibrium points for p-nitrobenzaldehyde (PNB) dimer in four different configurations.

PNB dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117305
C	6	0.02478168	-1.10254896	0.03500383
C	6	1.23131478	-0.41665328	-0.02260136
C	6	1.19007099	0.97239947	-0.04906487
H	1	-2.16701913	1.47059393	0.07150730
H	1	-2.11564064	-1.04795659	0.11637816
H	1	2.1607852	-0.96627808	-0.04689876
H	1	2.11246991	1.54006934	-0.09635325
N	7	0.05430805	-2.57314062	0.05567755
O	8	-1.02379966	-3.16082001	0.08791073
O	8	1.15500903	-3.11810827	0.03817252
C	6	-0.05168004	3.12475657	-0.05133451
O	8	-1.06583869	3.79219365	-0.02035229
H	1	0.94321316	3.60415411	-0.11097953
C	6	-0.08400372	-1.74724817	3.61289287
C	6	1.13600528	-1.06409490	3.61390758
C	6	1.15560675	0.32296574	3.62002373
C	6	-0.06050561	1.00037181	3.62674785
C	6	-1.28777194	0.34975731	3.63013101
C	6	-1.28797555	-1.04013646	3.62211204
H	1	2.05534935	-1.63576031	3.60795712

H	1	2.07895708	0.88358158	3.61840034
H	1	-2.20111036	0.92626137	3.63715076
H	1	-2.22761869	-1.58085406	3.62208104
N	7	-0.04648366	2.47133827	3.62730432
O	8	1.048599	3.02724957	3.60542607
O	8	-1.13066995	3.04834223	3.64841199
C	6	-0.1103629	-3.22811937	3.59861946
O	8	0.88442117	-3.92478967	3.59640956
H	1	-1.12037241	-3.67863059	3.58802605

PNB dimer in *cis*-sandwich configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117305
C	6	0.02478168	-1.10254896	0.03500383
C	6	1.23131478	-0.41665328	-0.02260136
C	6	1.19007099	0.97239947	-0.04906487
H	1	-2.16701913	1.47059393	0.07150730
H	1	-2.11564064	-1.04795659	0.11637816
H	1	2.1607852	-0.96627808	-0.04689876
H	1	2.11246991	1.54006934	-0.09635325
N	7	0.05430805	-2.57314062	0.05567755
O	8	-1.02379966	-3.16082001	0.08791073
O	8	1.15500903	-3.11810827	0.03817252
C	6	-0.05168004	3.12475657	-0.05133451
O	8	-1.06583869	3.79219365	-0.02035229
H	1	0.94321316	3.60415411	-0.11097953
C	6	-0.033602	1.64410698	3.68369985
C	6	-1.23173916	0.92596388	3.74582100
C	6	-1.21003163	-0.46084723	3.77117324
C	6	0.02478168	-1.10254896	3.73500371
C	6	1.23131478	-0.41665328	3.67739868
C	6	1.19007099	0.97239947	3.65093517
H	1	-2.16701913	1.47059393	3.77150726
H	1	-2.11564064	-1.04795659	3.81637812
H	1	2.1607852	-0.96627808	3.65310121
H	1	2.11246991	1.54006934	3.60364676
N	7	0.05430805	-2.57314062	3.75567746

O	8	-1.02379966	-3.16082001	3.7879107
O	8	1.15500903	-3.11810827	3.73817253
C	6	-0.05168004	3.12475657	3.64866543
O	8	-1.06583869	3.79219365	3.67964768
H	1	0.94321316	3.60415411	3.58902049

PNB dimer in T-shaped configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117305
C	6	0.02478168	-1.10254896	0.03500383
C	6	1.23131478	-0.41665328	-0.02260136
C	6	1.19007099	0.97239947	-0.04906487
H	1	-2.16701913	1.47059393	0.07150730
H	1	-2.11564064	-1.04795659	0.11637816
H	1	2.1607852	-0.96627808	-0.04689876
H	1	2.11246991	1.54006934	-0.09635325
N	7	0.05430805	-2.57314062	0.05567755
O	8	-1.02379966	-3.16082001	0.08791073
O	8	1.15500903	-3.11810827	0.03817252
C	6	-0.05168004	3.12475657	-0.05133451
O	8	-1.06583869	3.79219365	-0.02035229
H	1	0.94321316	3.60415411	-0.11097953
C	6	0.01096136	-0.06886557	8.13452339
C	6	0.0259201	1.14027703	7.43247509
C	6	0.0169307	1.13842499	6.04529238
C	6	-0.00880557	-0.08783601	5.38690424
C	6	-0.02834013	-1.30467618	6.05654001
C	6	-0.01716258	-1.28341413	7.44624949
H	1	0.04637834	2.0682056	7.98975468
H	1	0.03054382	2.05284023	5.47037649
H	1	-0.04979254	-2.22666001	5.49433136
H	1	-0.02940125	-2.21445107	8.00152016
N	7	-0.01250733	-0.09664917	3.91590214
O	8	0.0238369	0.98924112	3.34297657
O	8	-0.05050159	-1.18924749	3.35588074
C	6	0.02822374	-0.07243063	9.61559296
O	8	0.04631019	0.93291587	10.29669571

H	1	0.02533037	-1.07537103	10.08174038

PNB dimer in parallel-displaced configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117305
C	6	0.02478168	-1.10254896	0.03500383
C	6	1.23131478	-0.41665328	-0.02260136
C	6	1.19007099	0.97239947	-0.04906487
H	1	-2.16701913	1.47059393	0.07150730
H	1	-2.11564064	-1.04795659	0.11637816
H	1	2.1607852	-0.96627808	-0.04689876
H	1	2.11246991	1.54006934	-0.09635325
N	7	0.05430805	-2.57314062	0.05567755
O	8	-1.02379966	-3.16082001	0.08791073
O	8	1.15500903	-3.11810827	0.03817252
C	6	-0.05168004	3.12475657	-0.05133451
O	8	-1.06583869	3.79219365	-0.02035229
H	1	0.94321316	3.60415411	-0.11097953
C	6	-0.08400372	-2.94724822	3.71289301
C	6	1.13600528	-2.26409507	3.71390748
C	6	1.15560675	-0.87703431	3.72002363
C	6	-0.06050561	-0.19962825	3.72674775
C	6	-1.28777194	-0.85024267	3.73013091
C	6	-1.28797555	-2.24013638	3.72211194
H	1	2.05534935	-2.83576035	3.70795727
H	1	2.07895708	-0.31641844	3.71840024
H	1	-2.20111036	-0.27373865	3.73715091
H	1	-2.22761869	-2.78085399	3.72208118
N	7	-0.04648366	1.27133822	3.72730422
O	8	1.048599	1.82724953	3.70542598
O	8	-1.13066995	1.84834206	3.74841189
C	6	-0.1103629	-4.42811918	3.69861937
O	8	0.88442117	-5.12478971	3.69640946
H	1	-1.12037241	-4.87863016	3.68802595

TABLE S4. Cartesian coordinates at equilibrium points for p-nitrobenzaldehyde(PNB)-acetone in four different configurations.

PNB-acetone dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.084004	-1.74724805	3.71289301
C	6	1.13600504	-1.06409478	3.71390796
C	6	1.15560651	0.32296583	3.72002411
C	6	-0.06050586	1.00037193	3.72674799
C	6	-1.28777218	0.34975743	3.73013091
C	6	-1.28797579	-1.04013634	3.72211170
H	1	2.05534911	-1.63576019	3.70795774
H	1	2.07895684	0.88358164	3.71840119
H	1	-2.2011106	0.92626148	3.73715067
H	1	-2.22761893	-1.58085394	3.72208071
N	7	-0.04648391	2.47133827	3.7273047
O	8	1.04859877	3.02724981	3.70542645
O	8	-1.13067019	3.04834223	3.74841189
C	6	-0.11036319	-3.22811913	3.6986196
O	8	0.88442081	-3.92478967	3.69640994
H	1	-1.12037265	-3.67863035	3.68802595
PNB-acetone dimer in *cis*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550

C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.033602	1.64410698	3.58369994
C	6	-1.23173916	0.92596388	3.64582109
C	6	-1.21003163	-0.46084723	3.67117286
C	6	0.02478168	-1.10254896	3.63500381
C	6	1.23131478	-0.41665328	3.57739854
C	6	1.19007099	0.97239947	3.55093503
H	1	-2.16701913	1.47059393	3.67150736
H	1	-2.11564064	-1.04795659	3.71637821
H	1	2.1607852	-0.96627808	3.55310130
H	1	2.11246991	1.54006934	3.50364661
N	7	0.05430805	-2.57314062	3.65567756
O	8	-1.02379966	-3.16082001	3.68791056
O	8	1.15500903	-3.11810827	3.63817263
C	6	-0.05168004	3.12475657	3.54866552
O	8	-1.06583869	3.79219365	3.57964754
H	1	0.94321316	3.60415411	3.48902059

PNB-acetone dimer in linear configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.08279467	-0.10084683	0.05917428
O	8	-0.05791965	-1.33156693	0.04822838
C	6	1.18652391	0.71865851	0.10025407
C	6	-1.38438761	0.66715783	0.03180335
H	1	-2.22420788	-0.02694975	0.19718052
H	1	-1.37763679	1.46639562	0.80255550
H	1	-1.49207497	1.15966034	-0.95893300
H	1	2.05375934	0.06182724	-0.07489625
H	1	1.27340901	1.19988787	1.09832191
H	1	1.1476779	1.52874255	-0.65800649
C	6	-0.033602	8.84528065	-0.01630000
C	6	-1.23173857	8.12713623	0.04582098
C	6	-1.21002984	6.74032497	0.07117288

C	6	0.0247841	6.09862471	0.03500356
C	6	1.23131657	6.78452158	-0.02260161
C	6	1.19007158	8.17357445	-0.04906497
H	1	-2.16701913	8.67176533	0.07150734
H	1	-2.11563826	6.15321493	0.11637796
H	1	2.16078758	6.23489714	-0.04689910
H	1	2.11246991	8.74124527	-0.09635334
N	7	0.05431177	4.62803316	0.05567713
O	8	-1.02379549	4.04035282	0.08791029
O	8	1.1550132	4.08306646	0.03817201
C	6	-0.05168134	10.3259306	-0.05133436
O	8	-1.06584048	10.99336624	-0.02035205
H	1	0.94321144	10.80532837	-0.11097936

PNB-acetone dimer in parallel-displaced configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.033602	3.24410701	3.58369994
C	6	-1.23173916	2.52596402	3.64582109
C	6	-1.21003163	1.13915277	3.67117286
C	6	0.02478168	0.49745110	3.63500381
C	6	1.23131478	1.18334675	3.57739854
C	6	1.19007099	2.57239962	3.55093503
H	1	-2.16701913	3.07059407	3.67150736
H	1	-2.11564064	0.55204344	3.71637821
H	1	2.1607852	0.63372195	3.55310130
H	1	2.11246991	3.14006948	3.50364661
N	7	0.05430805	-0.97314066	3.65567756
O	8	-1.02379966	-1.56081998	3.68791056
O	8	1.15500903	-1.51810837	3.63817263

C	6	-0.05168004	4.72475672	3.54866552
O	8	-1.06583869	5.39219379	3.57964754
H	1	0.94321316	5.20415401	3.48902059

TABLE S5. Cartesian coordinates at equilibrium points for p-nitrobenzaldehyde (PNB)-hexane in four different configurations.

PNB-hexane dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	1.80318117	0.02855136	-3.70364118
C	6	1.11072814	-1.18617892	-3.71143746
C	6	-0.27645504	-1.19517601	-3.71229768
C	6	-0.94457102	0.02607166	-3.7069664
C	6	-0.28461704	1.24834049	-3.70338488
C	6	1.10525823	1.23790467	-3.70078278
H	1	1.67537165	-2.10986519	-3.71483302
H	1	-0.84409857	-2.114218	-3.71563721

H	1	-0.8541491	2.16606665	-3.70108628
H	1	1.65313506	2.17337728	-3.69558549
N	7	-2.41559291	0.02324891	-3.70189714
O	8	-2.97976661	-1.06770849	-3.68633008
O	8	-2.98437357	1.11192596	-3.71236134
C	6	3.28425431	0.04352865	-3.69493723
O	8	3.97330785	-0.95651537	-3.70314455
H	1	3.74250627	1.04996765	-3.67828131

PNB-hexane dimer in cross configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-0.033602	1.64410698	3.78369999
C	6	-1.23173916	0.92596388	3.84582114
C	6	-1.21003163	-0.46084723	3.87117314
C	6	0.02478168	-1.10254896	3.83500385
C	6	1.23131478	-0.41665328	3.77739859
C	6	1.19007099	0.97239947	3.75093508
H	1	-2.16701913	1.47059393	3.87150717
H	1	-2.11564064	-1.04795659	3.91637826

H	1	2.1607852	-0.96627808	3.75310111
H	1	2.11246991	1.54006934	3.70364666
N	7	0.05430805	-2.57314062	3.8556776
O	8	-1.02379966	-3.16082001	3.88791084
O	8	1.15500903	-3.11810827	3.83817244
C	6	-0.05168004	3.12475657	3.74866533
O	8	-1.06583869	3.79219365	3.77964759
H	1	0.94321316	3.60415411	3.6890204

PNB-hexane dimer in T-shaped configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-0.06233003	0.03278028	-8.11263275
C	6	-1.26833355	0.0513114	-7.4052906
C	6	-1.26060188	0.03391496	-6.0182085
C	6	-0.03164908	-0.0003097	-5.3652482
C	6	1.1823529	-0.01518177	-6.04013443
C	6	1.15513086	0.00082757	-7.42969227
H	1	-2.19857287	0.07734746	-7.95846987
H	1	-2.17255664	0.04479647	-5.43934059

H	1	2.1067102	-0.04008803	-5.48197985
H	1	2.08372045	-0.01244288	-7.98902273
N	7	-0.01683223	-0.02484776	-3.89449406
O	8	-1.10102141	-0.03000304	-3.3172338
O	8	1.07864249	-0.03978819	-3.33902097
C	6	-0.0653441	0.04348224	-9.59376621
O	8	-1.07334411	0.07723179	-10.2703352
H	1	0.93508697	0.01640272	-10.06450558

PNB-hexane dimer in parallel-displaced configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	2.10318112	0.02855136	-3.70364118
C	6	1.41072822	-1.18617892	-3.71143746
C	6	0.02354494	-1.19517601	-3.71229768
C	6	-0.64457107	0.02607166	-3.7069664
C	6	0.01538296	1.24834049	-3.70338488
C	6	1.40525818	1.23790467	-3.70078278
H	1	1.9753716	-2.10986519	-3.71483302
H	1	-0.54409856	-2.114218	-3.71563721

H	1	-0.55414903	2.16606665	-3.70108628
H	1	1.95313501	2.17337728	-3.69558549
N	7	-2.11559296	0.02324891	-3.70189714
O	8	-2.67976642	-1.06770849	-3.68633008
O	8	-2.68437362	1.11192596	-3.71236134
C	6	3.5842545	0.04352865	-3.69493723
O	8	4.27330732	-0.95651537	-3.70314455
H	1	4.04250622	1.04996765	-3.67828131

TABLE S6. Cartesian coordinates at equilibrium points for p-nitrobenzaldehyde (PNB)-silanol in five different configurations.

PNB-silanol dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
Si	14	-0.00687177	-0.54508191	3.83212805
O	8	0.00502312	1.10882843	3.92028499
H	1	-1.21073496	-1.04529309	3.13234758
H	1	0.03155539	-1.16247976	5.17620516
H	1	1.20211661	-0.90869278	3.0758729
H	1	-0.71340752	1.54358304	4.38102722

PNB-silanol dimer in *cis*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
Si	14	-0.01146683	0.55444044	3.83347726
O	8	-0.05298518	-1.10127425	3.81871843
H	1	1.19814587	1.07569063	3.15944004
H	1	-0.03269059	1.08755589	5.21352720
H	1	-1.21701527	0.98593217	3.10804248
H	1	0.6594829	-1.57661355	4.24752998
PNB-silanol dimer in linear (1) configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331

N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
Si	14	-0.02931391	-6.29414415	-0.00377521
O	8	-0.02424956	-7.95041609	0.00461132
H	1	1.09525168	-5.74932718	-0.79606146
H	1	0.06527882	-5.74221897	1.36576164
H	1	-1.31026995	-5.90649748	-0.61587834
H	1	0.73914993	-8.39973545	0.36898831

PNB-silanol dimer in linear (2) configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
Si	14	-0.00687177	6.95491791	-0.06787180
O	8	0.00502312	8.60882854	0.02028517
H	1	-1.21073496	6.45470667	-0.76765239
H	1	0.03155539	6.33752012	1.27620542
H	1	1.20211661	6.59130716	-0.8241272
H	1	-0.71340752	9.04358292	0.4810271

PNB-silanol dimer in T-shaped configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.0671961	0.02053264	1.73791921
C	6	1.14079487	0.00704111	1.03386140
C	6	1.13650882	0.00708989	-0.35334459
C	6	-0.09099697	0.02251488	-1.00973237
C	6	-1.30676389	0.04033528	-0.33810261
C	6	-1.28305292	0.03821080	1.05161035
H	1	2.06977201	-0.00523411	1.58963203
H	1	2.04998875	-0.00569681	-0.92976433
H	1	-2.22980976	0.05360233	-0.89881927
H	1	-2.2131815	0.04941431	1.60842288
N	7	-0.10236207	0.01670206	-2.48071027
O	8	0.98270673	-0.01795317	-3.05529451
O	8	-1.19609857	0.04567974	-3.03904676
C	6	-0.06812438	0.01278881	3.21907306
O	8	0.93847108	0.00406584	3.89851356
H	1	-1.07026243	0.01371753	3.68695164
Si	14	0.04698287	-0.56340873	7.07712793
O	8	-0.01601957	1.09148359	7.05076361
H	1	1.22745275	-1.07594347	6.34706640
H	1	-1.16229618	-1.16423821	6.47227383
H	1	0.13559622	-0.93237406	8.49902821
H	1	-0.07598723	1.5295409	6.20108891

TABLE S7. Cartesian coordinates at equilibrium points for p-nitrobenzaldehyde (PNB)-propylamine in four different configurations.

PNB-propylamine dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493

H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
C	6	-0.13993451	1.95265615	3.89711452
C	6	0.52693677	0.58340853	3.84940410
C	6	-0.48673043	-0.55169493	3.95597100
N	7	0.06303596	-1.90412688	3.91899276
H	1	-0.68678081	2.08591866	4.83103609
H	1	-0.85032099	2.06736565	3.07784796
H	1	0.58918822	2.75793338	3.82059407
H	1	-1.21291554	-0.46444827	3.14448857
H	1	-1.05052102	-0.44601154	4.88571596
H	1	1.08786893	0.47152942	2.91754699
H	1	1.25072706	0.48999804	4.66360474
H	1	0.72788608	-2.03167534	4.67347097
H	1	0.57713336	-2.04880023	3.05742478

PNB-propylamine dimer in *cis*-sandwich configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230

C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
C	6	-0.21175505	-1.90127134	3.80539203
C	6	0.47049591	-0.53888398	3.78905630
C	6	-0.53679085	0.60668546	3.80859113
N	7	0.02772497	1.95346439	3.79476881
H	1	-0.8625955	-2.02005267	2.9386127
H	1	-0.82555431	-2.01750112	4.69911766
H	1	0.51288033	-2.71407652	3.79130888
H	1	-1.16688335	0.51814216	4.69662476
H	1	-1.20370173	0.51559782	2.94813347
H	1	1.13487196	-0.44159555	4.6519928
H	1	1.09796476	-0.44412774	2.89864945
H	1	0.60378563	2.08231091	2.97070336
H	1	0.63792413	2.08468604	4.59349537

PNB-propylamine dimer in linear configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
C	6	-0.13993451	-6.64734411	-0.00288539
C	6	0.52693677	-8.01659107	-0.05059590
C	6	-0.48673043	-9.15169430	0.05597094
N	7	0.06303596	-10.50412750	0.01899264

H	1	-0.68678081	-6.51408148	0.93103594
H	1	-0.85032099	-6.53263426	-0.82215202
H	1	0.58918822	-5.84206629	-0.07940608
H	1	-1.21291554	-9.06444836	-0.7555114
H	1	-1.05052102	-9.04601097	0.98571581
H	1	1.08786893	-8.12847042	-0.98245311
H	1	1.25072706	-8.11000252	0.76360458
H	1	0.72788608	-10.63167572	0.77347076
H	1	0.57713336	-10.6487999	-0.84257519

PNB-propylamine dimer in parallel-displaced configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.033602	1.64410698	-0.01630000
C	6	-1.23173916	0.92596388	0.04582101
C	6	-1.21003163	-0.46084723	0.07117299
C	6	0.02478168	-1.10254896	0.03500372
C	6	1.23131478	-0.41665328	-0.02260148
C	6	1.19007099	0.97239947	-0.04906493
H	1	-2.16701913	1.47059393	0.07150734
H	1	-2.11564064	-1.04795659	0.11637810
H	1	2.1607852	-0.96627808	-0.04689892
H	1	2.11246991	1.54006934	-0.09635331
N	7	0.05430805	-2.57314062	0.05567738
O	8	-1.02379966	-3.16082001	0.08791056
O	8	1.15500903	-3.11810827	0.03817230
C	6	-0.05168004	3.12475657	-0.05133445
O	8	-1.06583869	3.79219365	-0.02035218
H	1	0.94321316	3.60415411	-0.11097947
C	6	-0.21175505	-3.90127134	3.70539188
C	6	0.47049591	-2.53888392	3.68905640
C	6	-0.53679085	-1.39331460	3.70859122
N	7	0.02772497	-0.04653564	3.69476891
H	1	-0.8625955	-4.02005243	2.83861256
H	1	-0.82555431	-4.01750088	4.59911776
H	1	0.51288033	-4.71407652	3.69130874
H	1	-1.16688335	-1.4818579	4.59662485
H	1	-1.20370173	-1.48440218	2.84813356
H	1	1.13487196	-2.44159555	4.55199289
H	1	1.09796476	-2.44412756	2.79864931

H	1	0.60378563	0.08231089	2.87070346
H	1	0.63792413	0.0846861	4.49349499

TABLE S8. Cartesian coordinates at equilibrium points for acetone-hexane in three different configurations.

Acetone-hexane dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-0.01156624	0.11488955	3.79624176
O	8	-0.00549363	1.3457191	3.8170352
C	6	-1.30142164	-0.67237544	3.76569462
C	6	1.27066004	-0.68549097	3.79956555
H	1	2.12014818	-0.01773864	4.01615334
H	1	1.21336973	-1.5037359	4.54794884
H	1	1.40555763	-1.15511274	2.8010807
H	1	-2.14444351	0.01087671	3.5741663
H	1	-1.43995047	-1.17656708	4.7464447

H	1	-1.2524308	-1.46353769	2.98828435

Acetone-hexane dimer in linear (1) configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-0.01156624	5.11488962	-0.00375815
O	8	-0.00549363	6.34571934	0.01703516
C	6	-1.30142164	4.32762432	-0.0343055
C	6	1.27066004	4.31450939	-0.00043462
H	1	2.12014818	4.98226118	0.2161532
H	1	1.21336973	3.49626422	0.74794924
H	1	1.40555763	3.84488726	-0.99891937
H	1	-2.14444351	5.01087666	-0.22583377
H	1	-1.43995047	3.82343268	0.94644451
H	1	-1.2524308	3.53646231	-0.81171566

Acetone-hexane dimer in linear (2) configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900

C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-0.01156624	-4.88511038	-0.00375815
O	8	-0.00549363	-3.6542809	0.01703516
C	6	-1.30142164	-5.67237568	-0.0343055
C	6	1.27066004	-5.68549109	-0.00043462
H	1	2.12014818	-5.01773882	0.2161532
H	1	1.21336973	-6.50373554	0.74794924
H	1	1.40555763	-6.15511274	-0.99891937
H	1	-2.14444351	-4.98912334	-0.22583377
H	1	-1.43995047	-6.17656708	0.94644451
H	1	-1.2524308	-6.46353769	-0.81171566

TABLE S9. Cartesian coordinates at equilibrium points for acetone-silanol in four different configurations.

Acetone-silanol dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516

C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
Si	14	-0.0007245	0.58330631	3.44345689
O	8	0.00515579	-1.07275796	3.41608238
H	1	0.11931599	1.10639966	4.82228041
H	1	-1.23983383	1.13347125	2.85089684
H	1	1.16534019	0.99534422	2.64576864
H	1	-0.68734968	-1.53657365	3.88804436

Acetone-silanol dimer in linear configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
Si	14	-0.00623668	4.33654594	-0.00588236
O	8	-0.02095969	5.99262428	0.01690894
H	1	-0.49189013	3.76919603	1.27139831
H	1	1.35281229	3.80729222	-0.25503370
H	1	-0.90692621	3.94893289	-1.10328948
H	1	0.51224071	6.44187832	0.67364764

Acetone-silanol dimer in T-shaped configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516

C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
Si	14	0.01112336	-0.01293467	3.86717105
O	8	0.04693098	-0.02577630	5.52303505
H	1	-0.22861519	1.34759450	3.33738208
H	1	-1.04553747	-0.90340751	3.33827972
H	1	1.33506835	-0.49307203	3.44005823
H	1	-0.73581982	0.25926429	5.99578285
Acetone-silanol dimer in parallel-displaced configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
Si	14	-0.0007245	1.38330638	3.44345689
O	8	0.00515579	-0.27275798	3.41608238
H	1	0.11931599	1.90639973	4.82228041
H	1	-1.23983383	1.93347120	2.85089684
H	1	1.16534019	1.79534411	2.64576864
H	1	-0.68734968	-0.73657376	3.88804436

TABLE S10. Cartesian coordinates at equilibrium points for acetone-propylamine in three different configurations.

Acetone-propylamine dimer in *trans*-sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.13993451	1.95265615	3.79711461
C	6	0.52693677	0.58340853	3.74940395
C	6	-0.48673043	-0.55169493	3.85597086
N	7	0.06303596	-1.90412688	3.81899261
H	1	-0.68678081	2.08591866	4.73103571
H	1	-0.85032099	2.06736565	2.97784781
H	1	0.58918822	2.75793338	3.72059393
H	1	-1.21291554	-0.46444827	3.04448867
H	1	-1.05052102	-0.44601154	4.78571606
H	1	1.08786893	0.47152942	2.81754684
H	1	1.25072706	0.48999804	4.56360483
H	1	0.72788608	-2.03167534	4.57347107
H	1	0.57713336	-2.04880023	2.95742464
Acetone-propylamine dimer in linear configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451

H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.15868212	-8.02650928	-0.01686032
C	6	-0.6160472	-6.57338905	0.01620147
C	6	0.55905175	-5.60159636	-0.02960473
N	7	0.21536528	-4.18251133	-0.00205227
H	1	0.48685071	-8.24986267	0.83308625
H	1	0.40619123	-8.23523712	-0.92590147
H	1	-1.00224948	-8.71444416	0.01611658
H	1	1.14453399	-5.78558540	-0.93338513
H	1	1.22467101	-5.80012655	0.81359822
H	1	-1.27824557	-6.36912918	-0.82954717
H	1	-1.19789612	-6.38368893	0.92228425
H	1	-0.3120212	-3.96705031	0.83638179
H	1	-0.3863624	-3.95354652	-0.78501117

Acetone-propylamine dimer in parallel-displaced configuration

Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-0.01156624	0.11488955	-0.00375815
O	8	-0.00549363	1.34571910	0.01703516
C	6	-1.30142164	-0.67237544	-0.03430550
C	6	1.27066004	-0.68549097	-0.00043462
H	1	2.12014818	-0.01773864	0.21615320
H	1	1.21336973	-1.50373590	0.74794924
H	1	1.40555763	-1.15511274	-0.99891937
H	1	-2.14444351	0.01087671	-0.22583377
H	1	-1.43995047	-1.17656708	0.94644451
H	1	-1.2524308	-1.46353769	-0.81171566
C	6	-0.13993451	3.55265617	3.79711461
C	6	0.52693677	2.18340850	3.74940395
C	6	-0.48673043	1.04830503	3.85597086
N	7	0.06303596	-0.30412686	3.81899261
H	1	-0.68678081	3.68591881	4.73103571
H	1	-0.85032099	3.66736579	2.97784781
H	1	0.58918822	4.35793352	3.72059393
H	1	-1.21291554	1.13555169	3.04448867
H	1	-1.05052102	1.15398848	4.78571606
H	1	1.08786893	2.07152939	2.81754684
H	1	1.25072706	2.08999801	4.56360483
H	1	0.72788608	-0.43167537	4.57347107

H	1	0.57713336	-0.44880018	2.95742464

TABLE S11. Cartesian coordinates at equilibrium points for hexane-propylamine in linear configuration.

Hexane-propylamine dimer in linear configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
C	6	-1.9124428	0.3474696	3.72744846
C	6	-0.62413043	-0.46420807	3.78457189
C	6	0.61526549	0.4212864	3.70010304
N	7	1.89967227	-0.27207324	3.74737239
H	1	-1.97427726	0.91283792	2.79710245
H	1	-1.95958531	1.05966175	4.5518055
H	1	-2.79280186	-0.2906715	3.78820109
H	1	0.59722817	1.14626861	4.51713181
H	1	0.58262944	1.00047743	2.77439928
H	1	-0.58505189	-1.04124546	4.71248388

H	1	-0.59967339	-1.18745637	2.96491694
H	1	1.96371436	-0.94089758	2.98835754
H	1	1.9772805	-0.805556	4.60580063

TABLE S12. Cartesian coordinates at equilibrium points for hexane-silanol dimer in two different configurations.

Hexane-silanol dimer in sandwich configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
Si	14	-0.57636207	-0.01518897	3.95881033
O	8	1.0797199	-0.04123434	3.96566582
H	1	-1.10038912	1.15124559	3.21448708
H	1	-1.12605703	0.03265449	5.33167124
H	1	-0.98793107	-1.26218832	3.29443717
H	1	1.54325831	0.69789189	4.36096525

Hexane-silanol dimer in T-shaped configuration				
Atomic type	Atomic number	Coordinates x (Angstroms)	Coordinates y (Angstroms)	Coordinates z (Angstroms)
C	6	-3.19168711	0.22053400	-0.00007900
C	6	3.191679	-0.22064000	-0.00010900
C	6	-0.66249651	0.37542349	0.00008400
C	6	0.66248655	-0.37553293	0.00013870
C	6	1.87529767	0.54650563	0.00002184
C	6	-1.87530732	-0.54661465	-0.00003970
H	1	4.0495882	0.45090935	-0.00031807
H	1	-4.04959822	-0.45101309	-0.00015142
H	1	-3.26719499	0.85966712	-0.88042289
H	1	-3.26732731	0.85955530	0.88033670
H	1	3.26739216	-0.85962069	0.88033277
H	1	3.26711679	-0.85981274	-0.88042748
H	1	-1.82842422	-1.19997871	0.87536758
H	1	-1.82830048	-1.19987381	-0.87551820
H	1	1.82844031	1.19982517	0.87546831
H	1	1.8282634	1.19980919	-0.87541753
H	1	-0.70737624	1.03037131	-0.87630719
H	1	-0.7075243	1.03030610	0.87652022
H	1	0.70745343	-1.03037989	0.87660414
H	1	0.70742667	-1.03051639	-0.87622339
Si	14	-0.013387	0.04167768	3.7777946
O	8	-0.00490459	-0.01404535	5.43313599
H	1	-0.19010881	1.42359102	3.27952218
H	1	-1.09600782	-0.79201818	3.21027017
H	1	1.29710364	-0.48052168	3.35861659
H	1	-0.78321582	0.29034868	5.90112448

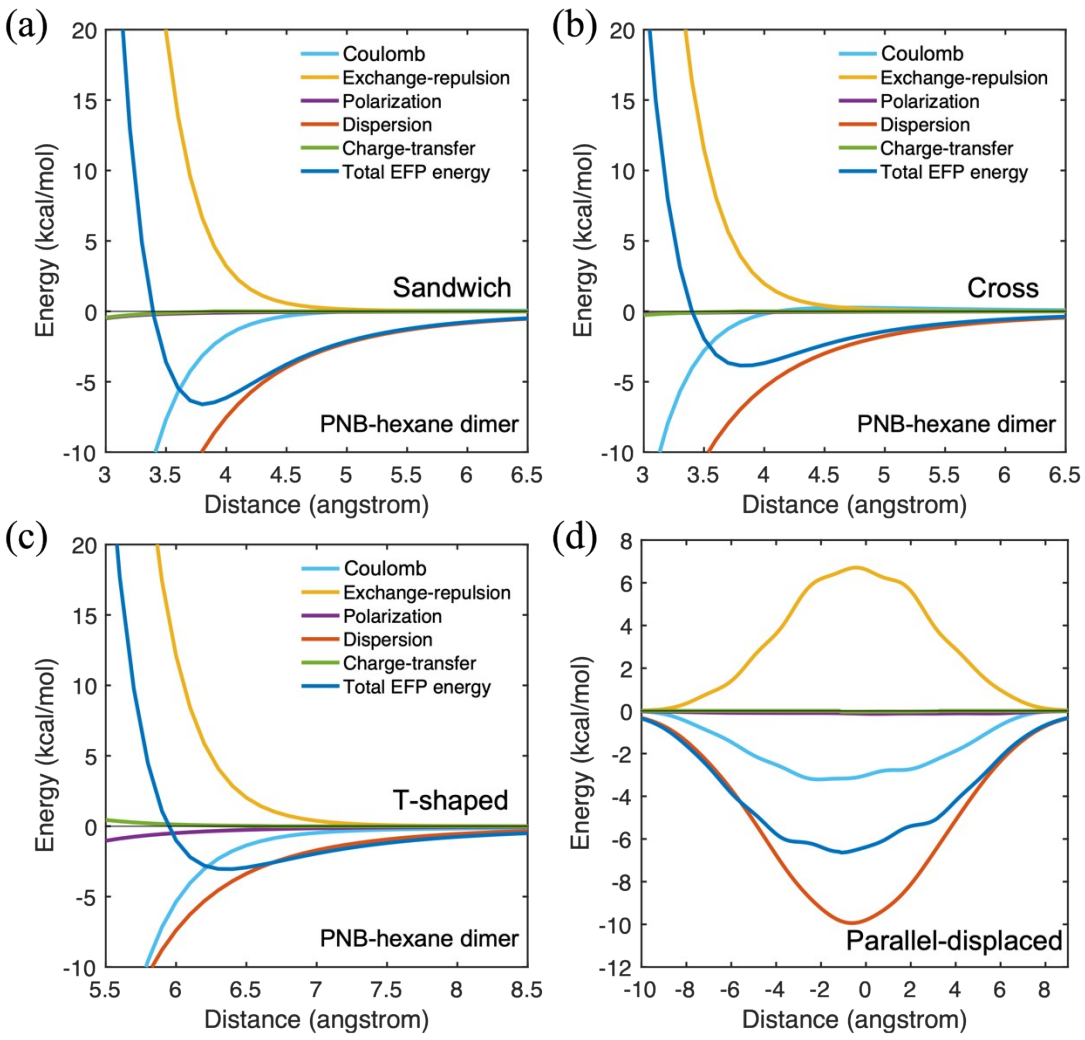

FIGURE S1. Potential energy surface for p-nitrobenzaldehyde (PNB)-hexane in four different configurations. (a) *trans*-Sandwich (b) Cross (c) T-shaped (d) Parallel-displaced

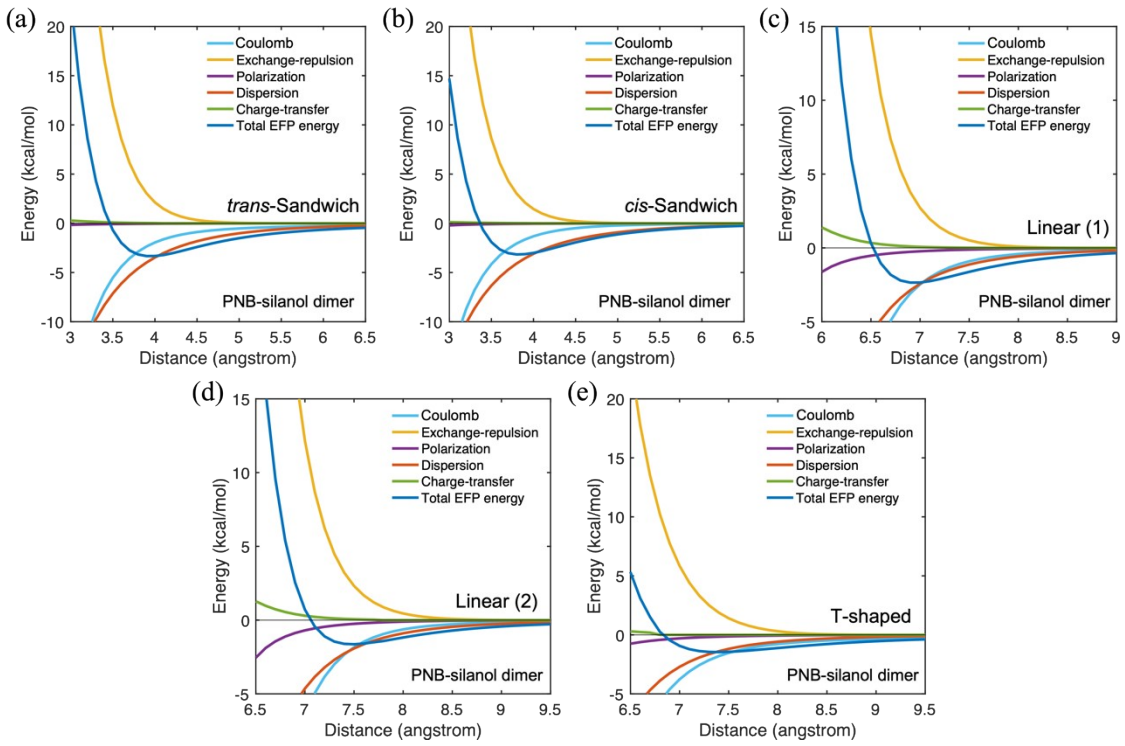

FIGURE S2. Potential energy surface for p-nitrobenzaldehyde (PNB)-silanol in five different configurations. (a) *trans*-Sandwich (b) *cis*-Sandwich (c) Linear (1) (d) Linear (2) (e) T-shaped

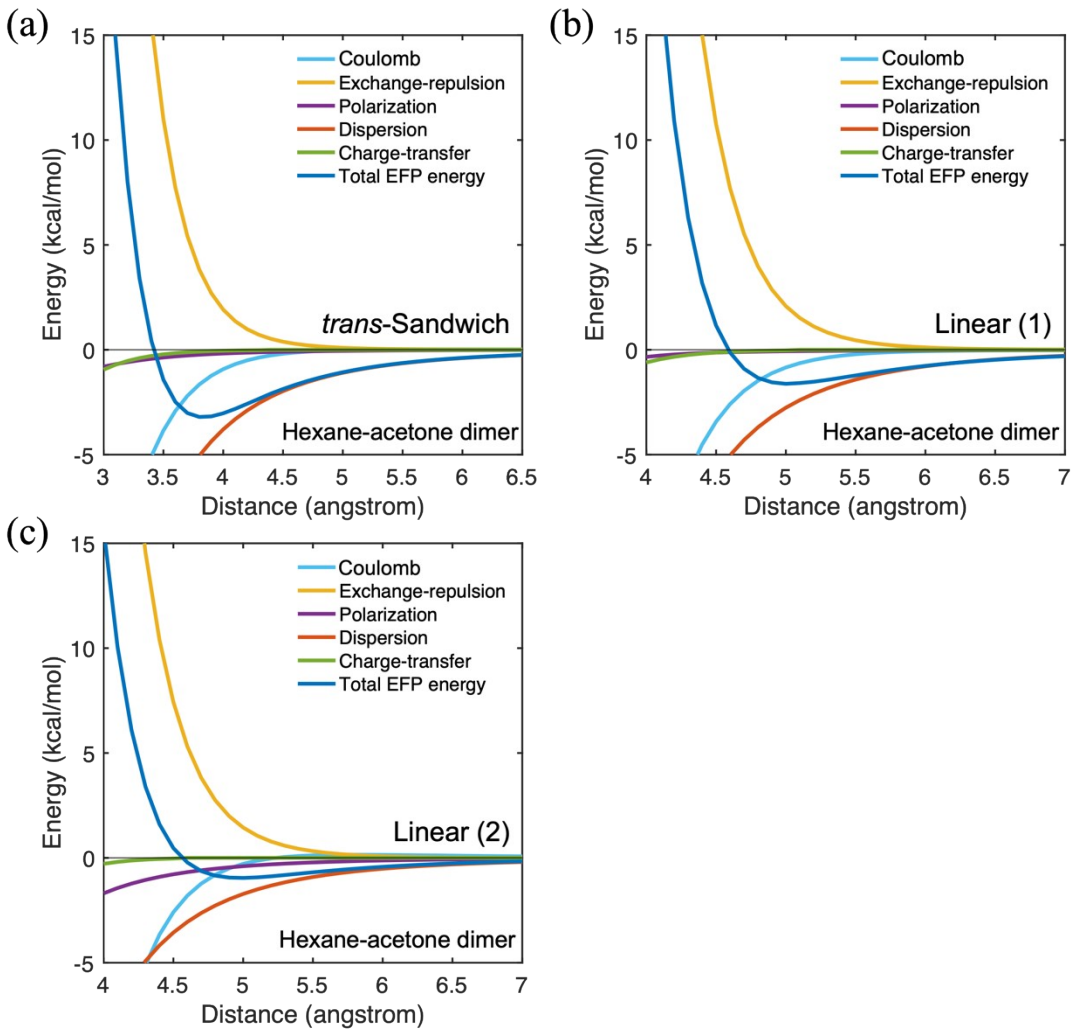

FIGURE S3. Potential energy surface for acetone-hexane in three different configurations. (a) *trans*-Sandwich (b) Linear (1) (c) Linear (2)

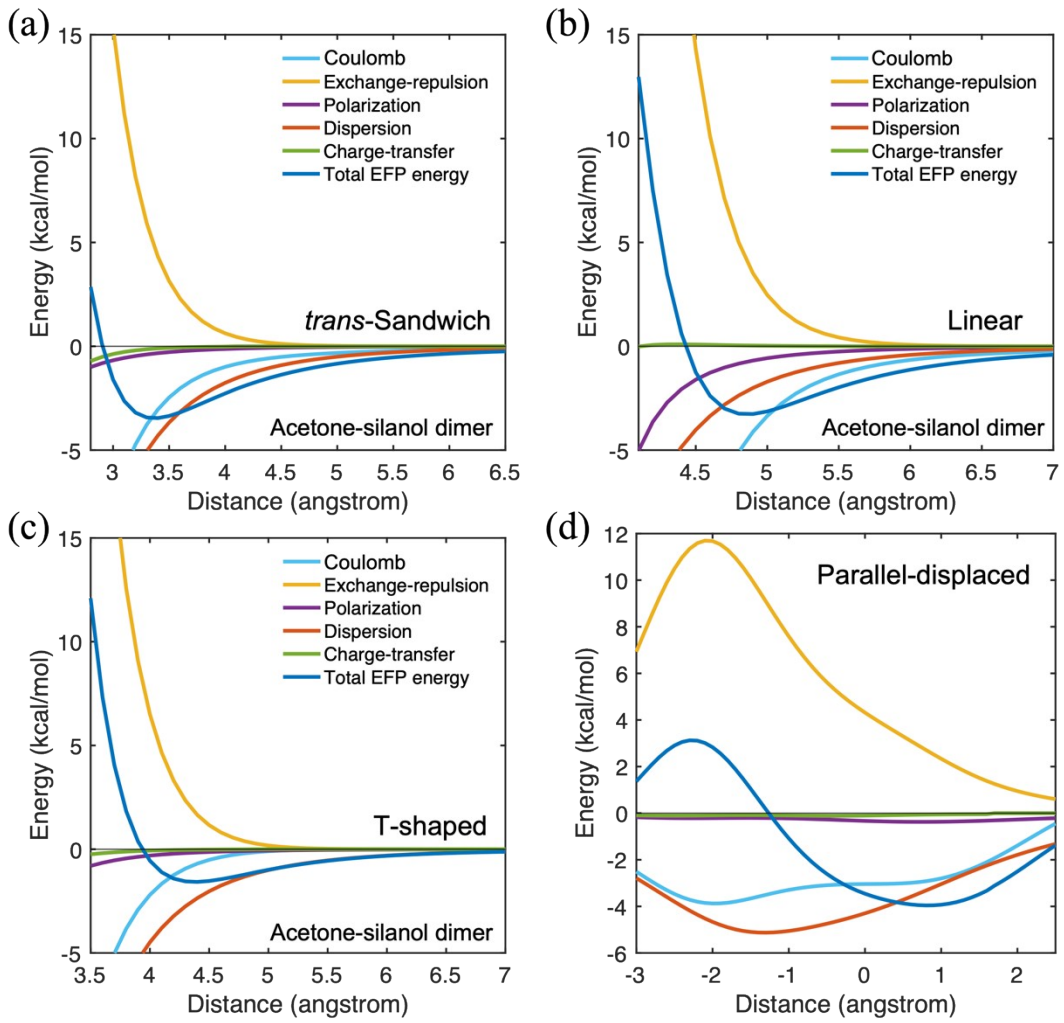

FIGURE S4. Potential energy surface for acetone-silanol in four different configurations. (a) *trans*-Sandwich (b) Linear (c) T-shaped (d) Parallel-displaced

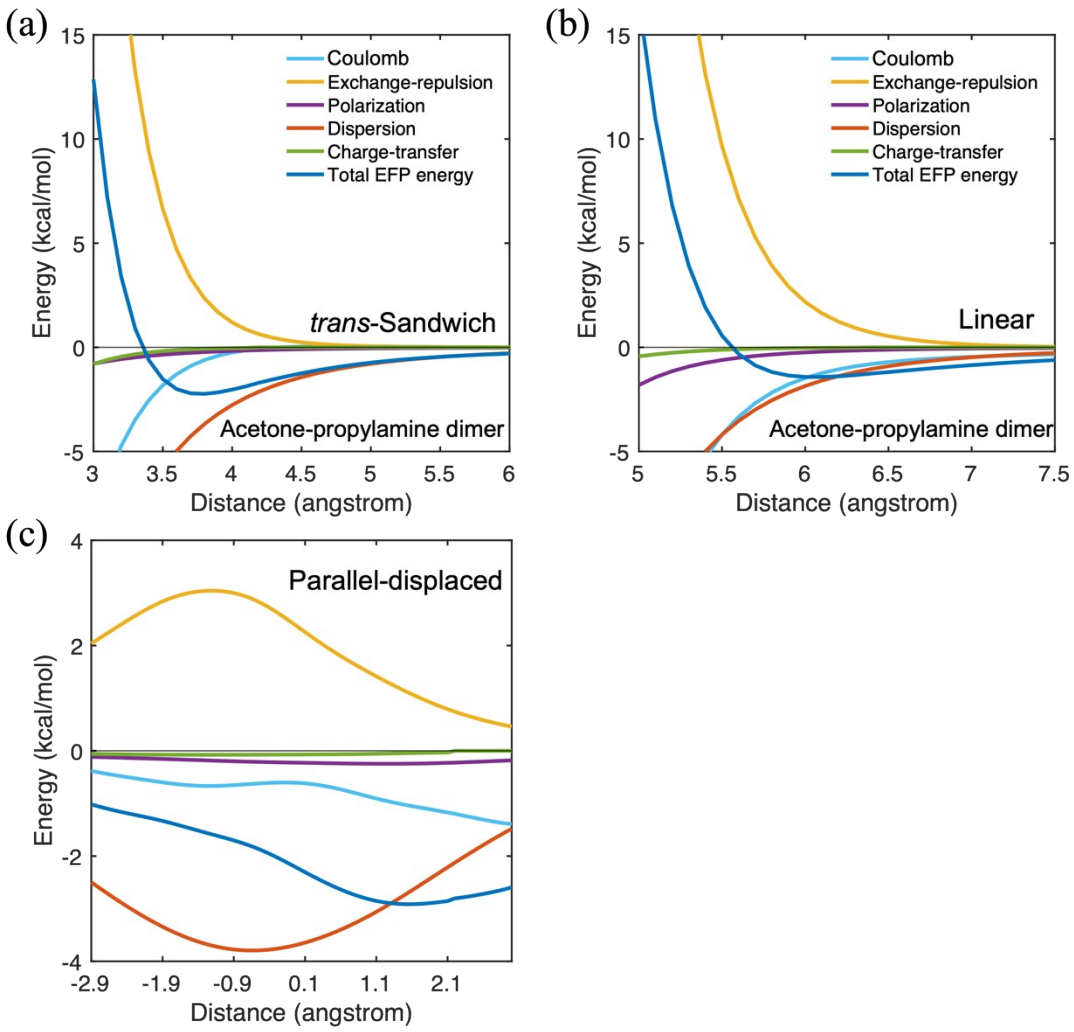

FIGURE S5. Potential energy surface for acetone-propylamine in three different configurations.

(a) *trans*-Sandwich (b) Linear (c) Parallel-displaced

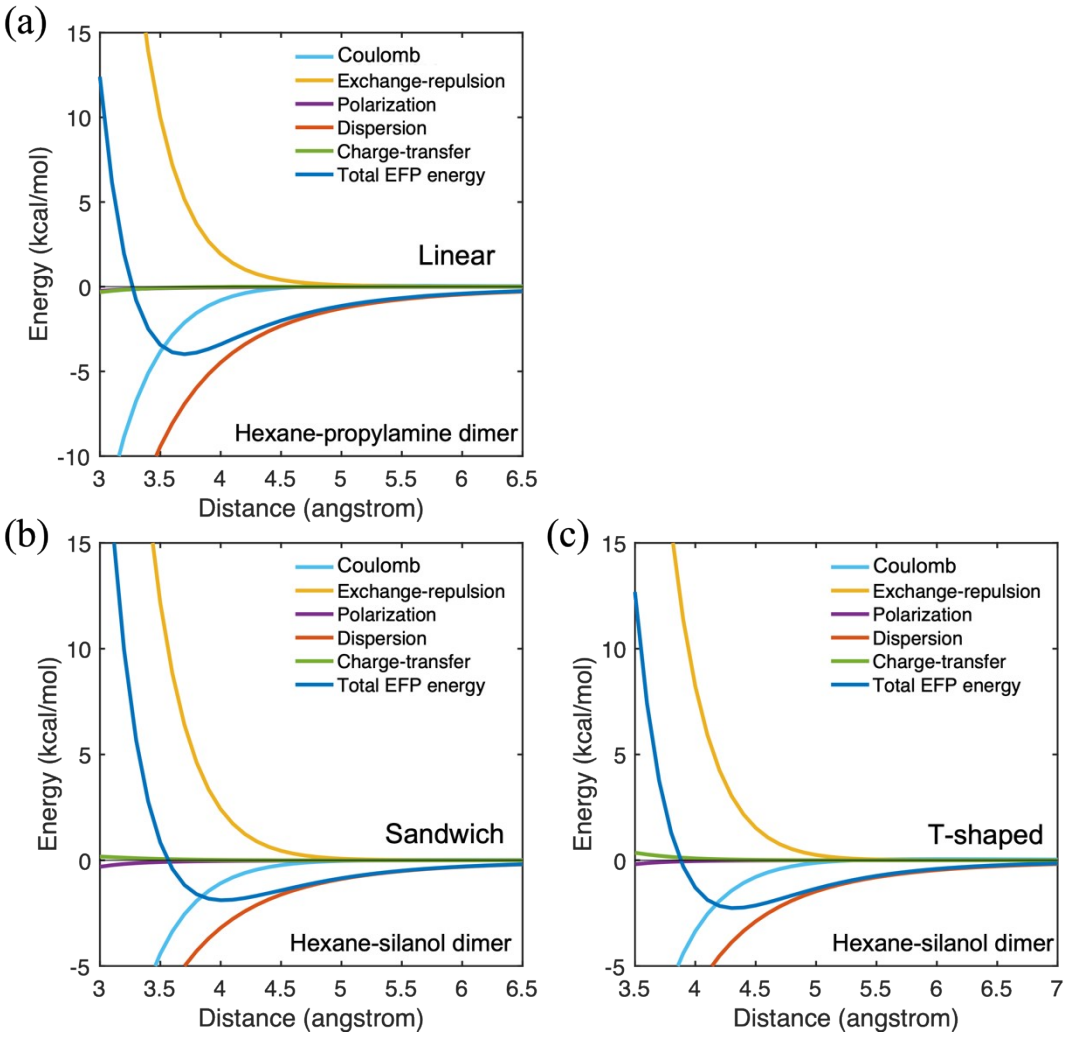

FIGURE S6. Potential energy surface (a) linear configuration for hexane-propylamine dimer (b) sandwich configuration for hexane-silanol dimer (c) T-shaped configuration for hexane-silanol dimer