

**Comment on "Theoretical studies on a carbonaceous molecular bearing:
association thermodynamics and dualmode rolling dynamics"**

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Supplementary Information

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Table S1. Calculated association free energy in dichloromethane, $\Delta G_{\text{solvent}}$. B97-D2/def2-TZVP geometries are used for the complexes. Single point calculations are performed with the def2-TZVP basis set. All values in kcal mol⁻¹.

	complex	ΔE_{comp}^a	$\Delta E_{\text{disp,3body}}$	Δ_{RRHO}^b	ΔG_{gas}^c	$\Delta G_{\text{solv. (SMD)}}$	$\Delta G_{\text{solv.}}$	dev ^e
B3LYP-D3	A	-62.10 (-86.80)	5.85	18.63	-37.62	25.40	-12.22	
	B	-62.72 (-86.28)	5.56	17.69	-39.47	25.65	-13.83	-0.83
B97-D2	A	-62.95 (-98.28)	5.85	18.63	-38.47	25.10	-13.37	
	B	-63.37 (-97.42)	5.56	17.69	-40.12	25.28	-14.83	-1.83
TPSS-D3	A	-58.22 (-78.53)	5.85	18.63	-33.74	25.06	-8.68	
	B	-58.88 (-77.99)	5.56	17.69	-35.63	25.24	-10.39	+2.61
B97-D3	A	-64.95 (-100.28)	5.85	18.63	-40.47	25.10	-15.36	
	B	-65.68 (-99.73)	5.56	17.69	-42.43	25.28	-17.14	-4.14

^a $\Delta E_{\text{complexation}}$ includes $\Delta E_{\text{dispersion}}$ contribution (in brackets).

^b Frequencies obtained at the PM6-D3 level.

^c $\Delta G_{\text{gas}} = \Delta E_{\text{comp}} + \Delta E_{\text{disp,3body}} + \Delta_{\text{RRHO}}$.

^d For B97-D2 a 3-body term equal to that of the other functionals is assumed.

^e Deviation relative to the experimental value of -13.0 kcal mol⁻¹ for complex B.⁸

Table S2. $\Delta G_{\text{solvent}}$ calculated with different implicit solvation models (in kcal mol⁻¹). LC-BLYP/6-311G* geometry is used, and to make a fair comparison, all single point calculations are performed with the same basis set, namely, the LC-BLYP/6-311G*.

	electrostatic	non-electrostatic terms ^a	total	
SMD	2.73	18.69	21.42	complex A
PCM (IEFPCM)	2.72 ^b	20.01	22.73	
CPCM/COSMO	3.35	20.01	23.36	
SMD	3.17	19.30	22.47	complex B
PCM (IEFPCM)	3.01	16.70	19.70	
CPCM/COSMO	3.90	16.70	20.60	

^a Dispersion, repulsion and cavitation energies. The SMD model includes implicitly the non-electrostatic terms of Truhlar and co-workers. For PCM and CPCM models, the non-electrostatic terms must be explicitly added through the READ option (keywords Dis, Rep, and Cav). Curiously, in the previous version of Gaussian (G03), the non-electrostatic terms are calculated as default.

^b 2.8 kcal mol⁻¹ is the value supplied by Isobe *et al.* as the PCM solvent effect.

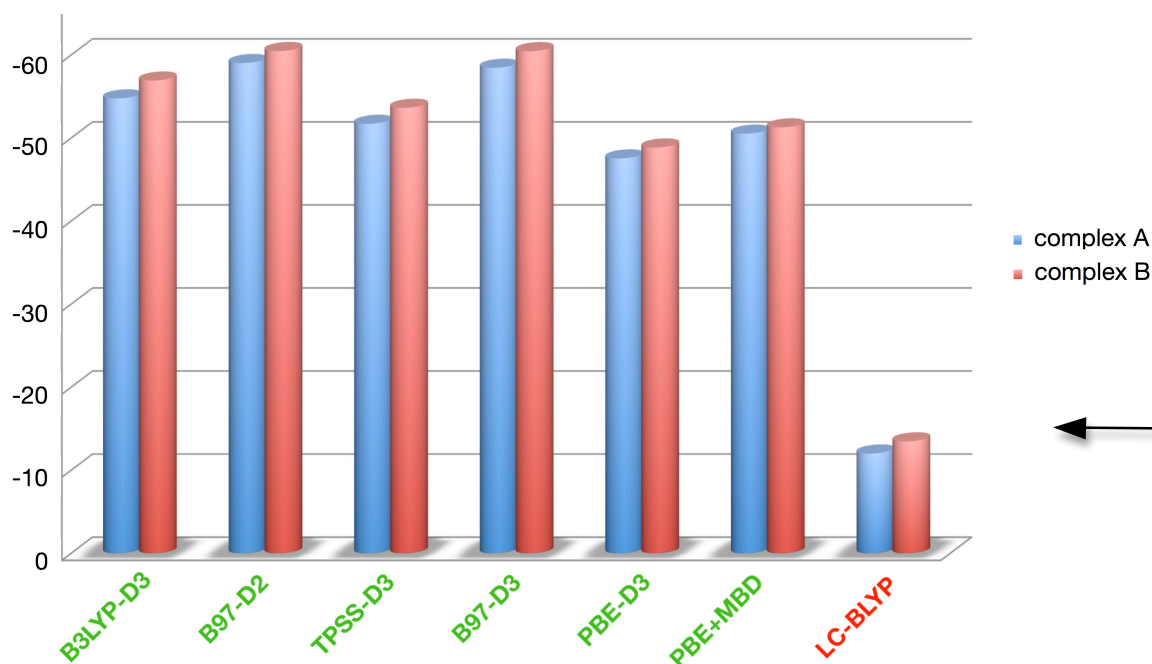
Table S3. Gas phase association energy (in kcal mol⁻¹). For DFT-D models it corresponds to $\Delta E_{\text{comp}} + \Delta E_{\text{disp,3body}}$, taken from Table 1 of the manuscript. LC-BLYP/6-311G* geometries are used.

B3LYP-D3	A	-54.77
	B	-56.92
B97-D2	A	-59.03
	B	-60.47
TPSS-D3	A	-51.71
	B	-53.64
B97-D3	A	-58.46
	B	-60.46
PBE-D3 ^a	A	-47.54
	B	-48.86
PBE+MBD ^b	A	-50.52
	B	-51.28
LC-BLYP	A	-12.01
	B	-13.47

^a Calculation with the TZP basis set. The D3 dispersion is -56.65 and -57.31 kcal mol⁻¹, for complex A and B, respectively. After adding $\Delta E_{\text{disp,3body}}$, these dispersions become -50.93 and -51.86 kcal mol⁻¹, respectively.

^b Calculation with the TZP basis set. The MBD dispersion is -53.91 and -54.28 kcal mol⁻¹, for complex A and B, respectively.

According to the above values of dispersion, and taking the Many Body Dispersion values as reference, it seems clear that the pairwise models from Grimme tend to overestimate dispersion effects in large systems. The addition of the three-body Axilrod-Teller contribution removes the overestimation but leads to an overcorrection, so that at the end the dispersion is underestimated. Therefore, this points to the need to go beyond the three-body contributions, including four-body contributions and more. In fact, the series only starts to converge with six-body contributions.¹⁴



Complex B (LC-BLYP/6-311G*)

C	5.541847	4.158322	-0.179813
C	4.861953	4.647059	-1.259396
C	3.788850	5.542386	-1.131608
C	3.370300	5.926798	0.143782
C	4.207236	5.585742	1.223135
C	5.258806	4.741486	1.068730
C	3.025149	5.943182	-2.277085
C	2.050161	6.476340	0.316873
C	1.253706	6.681926	-0.793015
C	1.820581	6.507426	-2.087715
C	-0.164842	6.852319	-0.619955
C	-0.718768	6.727046	0.654960
C	0.143740	6.715142	1.799660
C	1.471115	6.613964	1.610281
H	5.054921	4.236289	-2.240277
H	3.989327	5.958384	2.215063
H	5.850513	4.477040	1.936568
H	1.234591	6.764797	-2.960298
H	2.107943	6.555387	2.483421
C	-2.089056	6.443212	0.780603
H	-2.455619	6.173417	1.761131
C	-1.060356	6.952007	-1.702075
H	-0.689777	7.179474	-2.692523
C	-2.911288	6.319719	-0.302553
C	-2.384907	6.704385	-1.550444
H	-3.031103	6.752836	-2.418299
C	-4.175946	5.555501	-0.199096
C	-4.651020	4.870921	-1.281369
C	-4.774649	5.279212	1.043241
C	-5.546447	3.796817	-1.159339
H	-4.226566	5.059100	-2.257594
C	-5.619293	4.227269	1.192494
H	-4.520664	5.875631	1.911046
C	-5.946269	3.384373	0.113298
C	-5.928907	3.025058	-2.305538
H	-6.003837	4.013778	2.180833
C	-6.498874	2.065985	0.286907
C	-6.491866	1.819741	-2.116095
C	-6.684574	1.261865	-0.820530
C	-6.661792	1.496351	1.581759
H	-6.734486	1.226912	-2.988334
C	-6.849904	-0.156142	-0.640004
C	-6.756670	0.170169	1.779263
H	-6.625966	2.140354	2.450885
C	-6.739377	-0.700680	0.640677
C	-6.934290	-1.059510	-1.716348
C	-6.451604	-2.068970	0.779290
H	-7.150681	-0.696712	-2.712148
C	-6.686301	-2.382646	-1.551843
H	-6.194048	-2.427950	1.765998
C	-6.313245	-2.898925	-0.296765
H	-6.723291	-3.034281	-2.416007
C	6.313245	2.898925	-0.296765
C	6.451604	2.068970	0.779290
C	6.686301	2.382646	-1.551843
C	6.739377	0.700680	0.640677
H	6.194048	2.427950	1.765998
C	6.934290	1.059510	-1.716348
H	6.723291	3.034281	-2.416007
C	6.849904	0.156142	-0.640004
C	6.756670	-0.170169	1.779263
H	7.150681	0.696712	-2.712148
C	6.684574	-1.261865	-0.820530
C	6.661792	-1.496351	1.581759
C	6.498874	-2.065985	0.286907
C	6.491866	-1.819741	-2.116095
H	6.625966	-2.140354	2.450885
C	5.946269	-3.384373	0.113298
C	5.928907	-3.025058	-2.305538
H	6.734486	-1.226912	-2.988334
C	5.546447	-3.796817	-1.159339
C	5.619293	-4.227269	1.192494
C	4.651020	-4.870921	-1.281369
H	6.003837	-4.013778	2.180833
C	4.774649	-5.279212	1.043241
H	4.226566	-5.059100	-2.257594
C	4.175946	-5.555501	-0.199096
H	4.520664	-5.875631	1.911046
C	-5.541847	-4.158322	-0.179813
C	-4.861953	-4.647059	-1.259396
C	-5.258806	-4.741486	1.068730
C	-3.788850	-5.542386	-1.131608
H	-5.054921	-4.236289	-2.240277
C	-4.207236	-5.585742	1.223135
H	-5.850513	-4.477040	1.936568
C	-3.370300	-5.926798	0.143782
C	-3.025149	-5.943182	-2.277085
H	-3.989327	-5.958384	2.215063
C	-2.050161	-6.476340	0.316873
C	-1.820581	-6.507426	-2.087715
C	-1.253706	-6.681926	-0.793015
C	-1.471115	-6.613964	1.610281
H	-1.234591	-6.764797	-2.960298
C	0.164842	-6.852319	-0.619955
C	-0.143740	-6.715142	1.799660
H	-2.107943	-6.555387	2.483421
C	0.718768	-6.727046	0.654960
C	1.060356	-6.952007	-1.702075
C	2.089056	-6.443212	0.780603
H	0.689777	-7.179474	-2.692523
C	2.384907	-6.704385	-1.550444
H	2.455619	-6.173417	1.761131
C	2.911288	-6.319719	-0.302553
H	3.031103	-6.752836	-2.418299
C	5.641623	-3.530222	-3.682693
H	4.569472	-3.533247	-3.892822
H	6.003153	-4.550132	-3.822947
H	6.117903	-2.900661	-4.432643
C	3.537108	5.671214	-3.654568
H	3.537226	4.601329	-3.875953
H	4.559060	6.030647	-3.784991
H	2.913331	6.158365	-4.402367
C	-0.435094	6.729423	3.177089
H	-0.943267	5.788630	3.403439

H	-1.163669	7.531825	3.302756
H	0.345403	6.865841	3.923990
C	-5.641623	3.530222	-3.682693
H	-4.569472	3.533247	-3.892822
H	-6.003153	4.550132	-3.822947
H	-6.117903	2.900661	-4.432643
C	-6.794945	-0.399599	3.160170
H	-5.855796	-0.899818	3.409782
H	-7.594845	-1.132795	3.274576
H	-6.951934	0.385042	3.898659
C	-3.537108	-5.671214	-3.654568
H	-3.537226	-4.601329	-3.875953
H	-4.559060	-6.030647	-3.784991
H	-2.913331	-6.158365	-4.402367
C	0.435094	-6.729423	3.177089
H	0.943267	-5.788630	3.403439
H	1.163669	-7.531825	3.302756
H	-0.345403	-6.865841	3.923990
C	6.794945	0.399599	3.160170
H	5.855796	0.899818	3.409782
H	7.594845	1.132795	3.274576
H	6.951934	-0.385042	3.898659
C	-2.102498	1.126804	-2.198566
C	-1.069579	2.132403	-2.198954
C	0.193922	1.815998	-2.622096
C	-1.820903	-0.144781	-2.622237
C	-2.924515	1.332890	-1.032748
C	-2.400464	2.465655	-0.312698
C	-1.253706	2.960220	-1.033009
C	-0.164145	3.427412	-0.349660
C	1.341147	2.311038	-1.903248
C	1.820903	0.144781	-2.622237
C	2.102498	-1.126804	-2.198566
C	1.069579	-2.132403	-2.198954
C	-0.193922	-1.815998	-2.622096
C	-1.341147	-2.311038	-1.903248
C	-2.347460	-1.277840	-1.903266
C	-3.127576	-1.081483	-0.795446
C	-3.423261	0.256770	-0.349638
C	-2.401248	2.466388	1.055302
C	-2.923028	1.332521	1.775083
C	-3.420345	0.256787	1.091073
C	-3.124716	-1.080921	1.536876
C	-2.941471	-1.908269	0.370237
C	-1.986621	-2.886711	0.370429
C	-1.164872	-3.093878	-0.794766
C	0.164145	-3.427412	-0.349660
C	1.253706	-2.960220	-1.033009
C	2.347460	1.277840	-1.903266
C	2.923028	-1.332521	1.775083
C	3.420345	-0.256787	1.091073
C	3.124716	1.080921	1.536876
C	2.346426	1.277244	2.646151
C	1.820580	0.144872	3.366191
C	1.069069	-2.131258	2.941877
C	1.253212	-2.958796	1.775729
C	2.401248	-2.466388	1.055302
C	2.400464	-2.465655	-0.312698

C	2.924515	-1.332890	-1.032748
C	3.423261	-0.256770	-0.349638
C	2.941471	1.908269	0.370237
C	1.986621	2.886711	0.370429
C	1.164751	3.091799	1.536676
C	1.340541	2.310648	2.646227
C	0.194078	1.815711	3.366172
C	0.490789	0.477549	3.811107
C	-0.490789	-0.477549	3.811107
C	-0.194078	-1.815711	3.366172
C	0.163826	-3.424435	1.091409
C	-1.164751	-3.091799	1.536676
C	-1.340541	-2.310648	2.646227
C	-2.346426	-1.277244	2.646151
C	-1.820580	-0.144872	3.366191
C	-2.101494	1.126181	2.940890
C	-1.069069	2.131258	2.941877
C	-1.253212	2.958796	1.775729
C	-0.163826	3.424435	1.091409
C	3.127576	1.081483	-0.795446
C	1.164872	3.093878	-0.794766
C	2.101494	-1.126181	2.940890
C	-0.490718	-0.477507	-3.066286
C	0.490718	0.477507	-3.066286

Complex A (B97-D2/def2-TZVP)

C	-6.963977	1.021723	-0.064362
C	-6.561926	1.789591	1.024994
C	-6.011319	3.080758	0.877555
C	-5.833176	3.610000	-0.439206
C	-6.459443	2.915191	-1.507386
C	-7.014700	1.667872	-1.328872
C	-5.487558	3.798508	2.009453
C	-4.908011	4.699165	-0.642926
C	-4.291290	5.303115	0.482675
C	-4.688311	4.889365	1.790534
C	-3.143249	6.154828	0.283878
C	-2.574562	6.266370	-1.023683
C	-3.299736	5.765432	-2.160203
C	-4.443142	5.039966	-1.948480
H	-6.528316	1.336051	2.009167
H	-6.463558	3.342810	-2.505041
H	-7.438930	1.149323	-2.184708
H	-4.260252	5.382066	2.658332
H	-4.939042	4.619964	-2.818171
C	-1.240119	6.708978	-1.150970
H	-0.766497	6.613567	-2.121475
C	-2.429740	6.754708	1.355103
H	-2.881144	6.817898	2.340416
C	-0.467435	7.064640	-0.049742
C	-1.136897	7.201140	1.196576
H	-0.603259	7.602845	2.054269
C	1.003573	6.994858	-0.140878
C	1.740427	6.592078	0.969273
C	1.680745	7.039926	-1.388586
C	3.034049	6.038086	0.856894
H	1.258726	6.561935	1.940312

C	2.931972	6.482839	-1.533098	C	4.715452	-4.807379	1.865041
H	1.182482	7.459817	-2.258603	C	4.309223	-5.244823	0.567736
C	3.599478	5.860506	-0.445221	C	4.443253	-5.025114	-1.868839
C	3.718319	5.511696	2.008255	H	4.293288	-5.283750	2.744749
H	3.384371	6.483084	-2.519685	C	3.158034	-6.097541	0.392697
C	4.698813	4.941611	-0.618869	C	3.295518	-5.749932	-2.058886
C	4.812645	4.709707	1.818722	H	4.932798	-4.620883	-2.749531
C	5.264489	4.317470	0.522403	C	2.578332	-6.229594	-0.908195
C	5.093996	4.493450	-1.915535	C	2.452439	-6.677211	1.479961
H	5.278233	4.276962	2.699119	C	1.242142	-6.671858	-1.017111
C	6.119564	3.168714	0.343673	H	2.911723	-6.724183	2.462500
C	5.823618	3.350457	-2.111252	C	1.157679	-7.124114	1.339623
H	4.714498	5.003173	-2.795784	H	0.759841	-6.592999	-1.984926
C	6.274168	2.609662	-0.963466	C	0.478885	-7.008617	0.096490
C	6.687592	2.448606	1.427538	H	0.629671	-7.509458	2.208247
C	6.718741	1.275373	-1.085702	C	-3.132856	-5.595630	3.538300
H	6.719872	2.893141	2.417457	H	-2.166804	-5.081548	3.651872
C	7.145096	1.159034	1.273010	H	-2.961772	-6.658285	3.757652
H	6.653545	0.810404	-2.062824	H	-3.821254	-5.189631	4.287589
C	7.044945	0.495570	0.020096	C	-5.737496	3.306933	3.412801
H	7.525343	0.623850	2.139294	H	-5.239773	2.340449	3.583499
C	-7.033954	-0.446991	0.064629	H	-6.808836	3.155100	3.602234
C	-6.714080	-1.251725	-1.025158	H	-5.349900	4.022001	4.146729
C	-7.131639	-1.082303	1.332158	C	-2.755159	5.936254	-3.554878
C	-6.271289	-2.583800	-0.874660	H	-1.834079	5.348440	-3.684805
H	-6.653209	-0.808490	-2.012678	H	-2.503340	6.984348	-3.765393
C	-6.674995	-2.368580	1.513831	H	-3.482756	5.593420	-4.298471
H	-7.509245	-0.527602	2.187266	C	3.188629	5.762387	3.397583
C	-6.110896	-3.112539	0.444271	H	2.216210	5.268302	3.542087
C	-5.828182	-3.352726	-2.006834	H	3.035930	6.834257	3.583388
H	-6.705216	-2.791806	2.513145	H	3.881858	5.371782	4.150611
C	-5.252310	-4.254848	0.645748	C	6.059081	2.826299	-3.504717
C	-5.099299	-4.492087	-1.788026	H	5.481429	1.905855	-3.676340
C	-4.695080	-4.907948	-0.483315	H	7.116718	2.580740	-3.670417
C	-4.785149	-4.607071	1.947962	H	5.748539	3.564397	-4.252196
H	-4.726045	-5.023654	-2.657967	C	5.776263	-3.195723	3.450621
C	-3.592682	-5.820234	-0.294492	H	5.280503	-2.225781	3.606942
C	-3.684806	-5.397896	2.149082	H	6.848944	-3.041123	3.629903
H	-5.240810	-4.147763	2.820036	H	5.393418	-3.897033	4.200184
C	-3.013532	-5.958675	1.006398	C	2.736918	-5.939438	-3.445353
C	-2.934932	-6.472056	-1.371110	H	1.816419	-5.350151	-3.573011
C	-1.718276	-6.508195	1.121416	H	2.479680	-6.989543	-3.638549
H	-3.397710	-6.500987	-2.352495	H	3.457818	-5.609186	-4.201084
C	-1.681190	-7.022653	-1.223625	C	-6.071041	-2.861306	-3.410830
H	-1.226036	-6.448667	2.085795	H	-5.493704	-1.945575	-3.607118
C	-0.992579	-6.941780	0.015800	H	-7.129381	-2.618680	-3.576410
H	-1.189651	-7.465300	-2.086220	H	-5.765172	-3.616929	-4.142558
C	6.978172	-0.975738	-0.077646	C	1.196936	2.070228	2.143674
C	6.583180	-1.722330	1.028949	C	-0.246779	2.383051	2.138797
C	7.023549	-1.647248	-1.329192	C	-1.172029	1.449019	2.562028
C	6.032711	-3.016557	0.909796	C	1.649561	0.837604	2.572286
H	6.555305	-1.249779	2.004377	C	1.783875	2.695483	0.978837
C	6.467461	-2.897727	-1.480293	C	0.733769	3.387279	0.256803
H	7.443902	-1.145976	-2.197135	C	-0.513815	3.194342	0.970940
C	5.846414	-3.570957	-0.395439	C	-1.711730	3.038198	0.258301
C	5.516435	-3.712953	2.058294	C	-2.378244	1.256285	1.807614
H	6.466817	-3.345297	-2.469175	C	-1.664369	-0.848829	2.537279
C	4.918992	-4.662746	-0.572931	C	-1.213864	-2.076011	2.098292

C	0.228902	-2.388812	2.103605
C	1.144066	-1.457505	2.546645
C	2.361110	-1.255609	1.812097
C	2.672034	0.161405	1.825388
C	3.271065	0.759876	0.708126
C	2.814834	2.057018	0.274351
C	0.744862	3.415602	-1.139462
C	1.802546	2.737453	-1.867056
C	2.818395	2.071786	-1.172675
C	3.283079	0.775523	-1.633641
C	3.563822	-0.039825	-0.467515
C	3.265555	-1.403830	-0.479232
C	2.662201	-2.028960	0.683179
C	1.713865	-3.014951	0.229495
C	0.508590	-3.182196	0.926964
C	-2.683210	-0.162153	1.794632
C	-1.778573	-2.681591	-1.927409
C	-2.801948	-2.026542	-1.233223
C	-3.261751	-0.722944	-1.679100
C	-2.682837	-0.122947	-2.802433
C	-1.623381	-0.804188	-3.521159
C	0.240001	-2.369234	-3.085782
C	0.518905	-3.180959	-1.919871
C	-0.728320	-3.371681	-1.199454
C	-0.731595	-3.363895	0.197313
C	-1.788954	-2.682636	0.918543
C	-2.813224	-2.033905	0.213857
C	-3.553749	0.074460	-0.502922
C	-3.256660	1.438795	-0.491394
C	-2.655180	2.062625	-1.654264
C	-2.374744	1.297711	-2.790292
C	-1.125056	1.490638	-3.501264
C	-0.661184	0.192343	-3.953659
C	0.706666	-0.104468	-3.948960
C	1.165928	-1.409414	-3.511805
C	1.716040	-3.005247	-1.217294
C	2.676753	-2.010005	-1.658014
C	2.408191	-1.227513	-2.784846
C	2.716593	0.193186	-2.772383
C	1.664477	0.885499	-3.491336
C	1.217992	2.136009	-3.046367
C	-0.203480	2.443917	-3.051642
C	-0.494516	3.236225	-1.875540
C	-1.698855	3.050479	-1.188716
C	-3.272393	-0.743418	0.663092
C	-2.665837	2.046109	0.686662
C	-1.181378	-2.061217	-3.090375
C	0.775171	-0.179834	3.302138
C	1.091995	-0.281042	4.821610
H	1.887836	-1.004522	5.032954
C	-0.803570	0.162170	3.296871
C	-1.144178	0.202914	4.814128
H	-1.029847	1.244012	5.186188
H	-2.169169	-0.127335	5.018503
N	-0.168935	-0.690137	5.418239
C	-0.166690	-0.656843	6.871595
H	-1.147442	-0.972543	7.247950
H	0.593626	-1.348982	7.253791

H	0.051626	0.358444	7.265979
H	1.415381	0.715561	5.192664

Complex B (B97-D2/def2-TZVP)

C	-6.898017	0.963451	-0.106314
C	-6.519280	1.741236	0.984403
C	-5.984977	3.039401	0.837873
C	-5.798319	3.566518	-0.478807
C	-6.399014	2.857361	-1.551974
C	-6.939040	1.603408	-1.374567
C	-5.488220	3.770593	1.973346
C	-4.892098	4.672880	-0.675664
C	-4.295583	5.287512	0.454964
C	-4.701468	4.871550	1.759421
C	-3.159405	6.157345	0.265439
C	-2.586025	6.283796	-1.038903
C	-3.296126	5.773926	-2.181190
C	-4.426085	5.025415	-1.977773
H	-6.493866	1.293979	1.971587
H	-6.396660	3.280012	-2.551696
H	-7.346904	1.077364	-2.233611
H	-4.293390	5.374720	2.630748
H	-4.910092	4.600175	-2.851553
C	-1.258952	6.750319	-1.157835
H	-0.779401	6.667980	-2.126668
C	-2.459981	6.762555	1.343142
H	-2.915988	6.812700	2.326977
C	-0.496805	7.111928	-0.051217
C	-1.173560	7.230123	1.193050
H	-0.649660	7.633641	2.055847
C	0.975678	7.063174	-0.137034
C	1.713909	6.660647	0.972237
C	1.656348	7.126724	-1.382159
C	3.011406	6.115667	0.857718
H	1.230683	6.619234	1.942134
C	2.911919	6.580004	-1.528384
H	1.157410	7.551967	-2.249235
C	3.578090	5.948837	-0.444894
C	3.695267	5.580666	2.005531
H	3.367645	6.593143	-2.513401
C	4.671280	5.023961	-0.625992
C	4.785936	4.774802	1.809809
C	5.233015	4.387358	0.510352
C	5.059306	4.580556	-1.926406
H	5.250141	4.334165	2.686963
C	6.076284	3.231458	0.322483
C	5.776108	3.431007	-2.130854
H	4.682057	5.099232	-2.802421
C	6.221987	2.679059	-0.988853
C	6.639086	2.498167	1.400342
C	6.653545	1.341416	-1.120685
H	6.677129	2.935432	2.393254
C	7.083572	1.205268	1.236262
H	6.584202	0.885236	-2.101475
C	6.975798	0.551063	-0.021180
H	7.461067	0.662014	2.098514
C	-6.963814	-0.505138	0.026932

C	-6.647222	-1.313285	-1.061161	H	-5.387575	4.009346	4.110852
C	-7.065455	-1.138451	1.295455	C	-2.748934	5.962135	-3.572839
C	-6.214112	-2.648256	-0.909453	H	-1.811979	5.399820	-3.700643
H	-6.583295	-0.872712	-2.049448	H	-2.523862	7.017122	-3.779328
C	-6.620827	-2.428746	1.478468	H	-3.464013	5.602748	-4.320717
H	-7.438462	-0.580835	2.150484	C	3.167197	5.824614	3.396614
C	-6.062771	-3.179308	0.410133	H	2.194368	5.331170	3.539663
C	-5.771254	-3.417803	-2.040883	H	3.016365	6.895772	3.587630
H	-6.654495	-2.849816	2.478507	H	3.860160	5.428882	4.147023
C	-5.217653	-4.331289	0.613302	C	5.997629	2.910035	-3.527917
C	-5.053135	-4.563633	-1.820669	H	5.410359	1.995762	-3.699362
C	-4.660650	-4.986436	-0.514780	H	7.051680	2.655136	-3.702084
C	-4.763001	-4.695268	1.916891	H	5.689197	3.654076	-4.270346
H	-4.677520	-5.095178	-2.689648	C	5.794149	-3.185788	3.397418
C	-3.566849	-5.908555	-0.323178	H	5.287239	-2.225154	3.572538
C	-3.670086	-5.496074	2.120803	H	6.867729	-3.018143	3.558297
H	-5.222150	-4.238998	2.788671	H	5.434846	-3.899335	4.146862
C	-2.992857	-6.052000	0.979024	C	2.740097	-5.978734	-3.485575
C	-2.907560	-6.560370	-1.398603	H	1.802622	-5.418207	-3.617400
C	-1.695204	-6.596082	1.096171	H	2.513438	-7.037054	-3.672316
H	-3.369305	-6.591504	-2.380436	H	3.450743	-5.632673	-4.243901
C	-1.651595	-7.105506	-1.249482	C	-5.996787	-2.918529	-3.445145
H	-1.206449	-6.537182	2.062355	H	-5.412618	-2.005167	-3.631518
C	-0.963653	-7.019445	-0.009728	H	-7.051927	-2.669387	-3.621169
H	-1.157947	-7.547114	-2.111399	H	-5.687610	-3.672785	-4.176878
C	6.909718	-0.919589	-0.129981	C	1.339086	2.046331	2.184274
C	6.540974	-1.680583	0.975944	C	-0.052001	2.463151	2.171045
C	6.939674	-1.579450	-1.388414	C	-1.050785	1.583225	2.602978
C	6.005011	-2.980693	0.854226	C	1.680977	0.764741	2.630785
H	6.524441	-1.218375	1.956439	C	1.986903	2.604130	1.011412
C	6.398156	-2.835845	-1.541578	C	0.996763	3.367495	0.273688
H	7.340142	-1.067216	-2.259172	C	-0.264150	3.279022	0.989255
C	5.806980	-3.528350	-0.452340	C	-1.467176	3.180058	0.283470
C	5.517078	-3.693530	2.005138	C	-2.301009	1.484581	1.871337
H	6.387283	-3.273788	-2.534605	C	-1.726406	-0.667196	2.618708
C	4.900005	-4.638135	-0.624391	C	-1.378028	-1.956421	2.200090
C	4.726868	-4.796428	1.814947	C	0.012980	-2.373338	2.214760
C	4.310936	-5.233314	0.520431	C	1.005373	-1.485673	2.645430
C	4.426428	-5.013890	-1.917347	C	2.266169	-1.399962	1.930495
H	4.325229	-5.285185	2.697409	C	2.684217	-0.008729	1.921578
C	3.173250	-6.105697	0.353128	C	3.307044	0.527823	0.790308
C	3.295632	-5.766171	-2.100769	C	2.951555	1.857142	0.327431
H	4.905407	-4.604717	-2.801494	C	1.006655	3.353986	-1.123472
C	2.592366	-6.255611	-0.945448	C	2.005792	2.576176	-1.832660
C	2.480148	-6.691743	1.445420	C	2.959004	1.842034	-1.121666
C	1.264984	-6.724962	-1.048545	C	3.322442	0.506027	-1.555706
H	2.941563	-6.724037	2.427459	C	3.535080	-0.308378	-0.373523
C	1.193162	-7.162563	1.311020	C	3.131903	-1.646415	-0.364540
H	0.779941	-6.660525	-2.016029	C	2.485197	-2.203604	0.808406
C	0.509300	-7.067062	0.068644	C	1.455871	-3.124056	0.361301
H	0.674338	-7.550627	2.183918	C	0.242451	-3.210074	1.050873
C	-3.132717	-5.712733	3.512839	C	-2.719143	0.093354	1.881288
H	-2.158976	-5.216556	3.639101	C	-1.985645	-2.558307	-1.816035
H	-2.980618	-6.779884	3.724202	C	-2.949176	-1.811733	-1.132230
H	-3.820458	-5.301872	4.259912	C	-3.305987	-0.483728	-1.595335
C	-5.752753	3.284130	3.375584	C	-2.684048	0.052314	-2.727413
H	-5.243444	2.326709	3.560805	C	-1.681509	-0.720864	-3.437514
H	-6.824743	3.118127	3.548371	C	0.051298	-2.418294	-2.976620

C	0.263381	-3.233195	-1.794333
C	-0.997100	-3.323134	-1.078493
C	-1.007746	-3.311410	0.318657
C	-2.008496	-2.535147	1.028070
C	-2.963132	-1.800895	0.316968
C	-3.535800	0.351652	-0.431016
C	-3.132456	1.689578	-0.440167
C	-2.484392	2.245388	-1.613343
C	-2.266578	1.443437	-2.736870
C	-1.006350	1.528828	-3.452705
C	-0.645047	0.191585	-3.885575
C	0.695340	-0.210383	-3.872207
C	1.050077	-1.539631	-3.410080
C	1.465668	-3.134360	-1.088428
C	2.500947	-2.223156	-1.536820
C	2.299647	-1.441361	-2.677538
C	2.717256	-0.050305	-2.687038
C	1.725207	0.709993	-3.425342
C	1.376336	1.998455	-3.005823
C	-0.013854	2.415209	-3.020416
C	-0.243110	3.251093	-1.856015
C	-1.455538	3.164419	-1.166121
C	-3.325008	-0.463520	0.750675
C	-2.502960	2.267747	0.731796
C	-1.338982	-2.001604	-2.989946
C	0.644094	-0.147977	3.077750
C	-0.696095	0.253503	3.064462