-Supporting Information-

Synthesis, Structure and Dispersion Interactions in Bis(1,8-naphthalendiyl)distibine

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Content

Figure S1. ^{1}H NMR spectrum of **1** in $CDCl_3$ at room temperature.

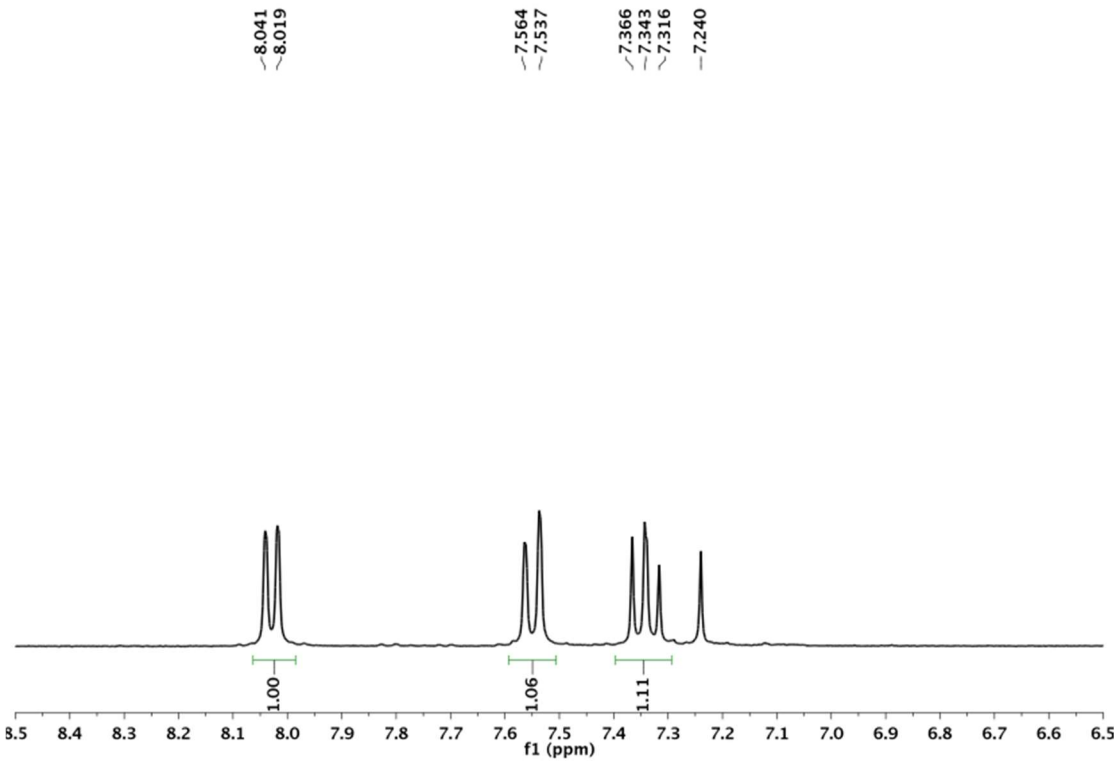


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$ at room temperature.

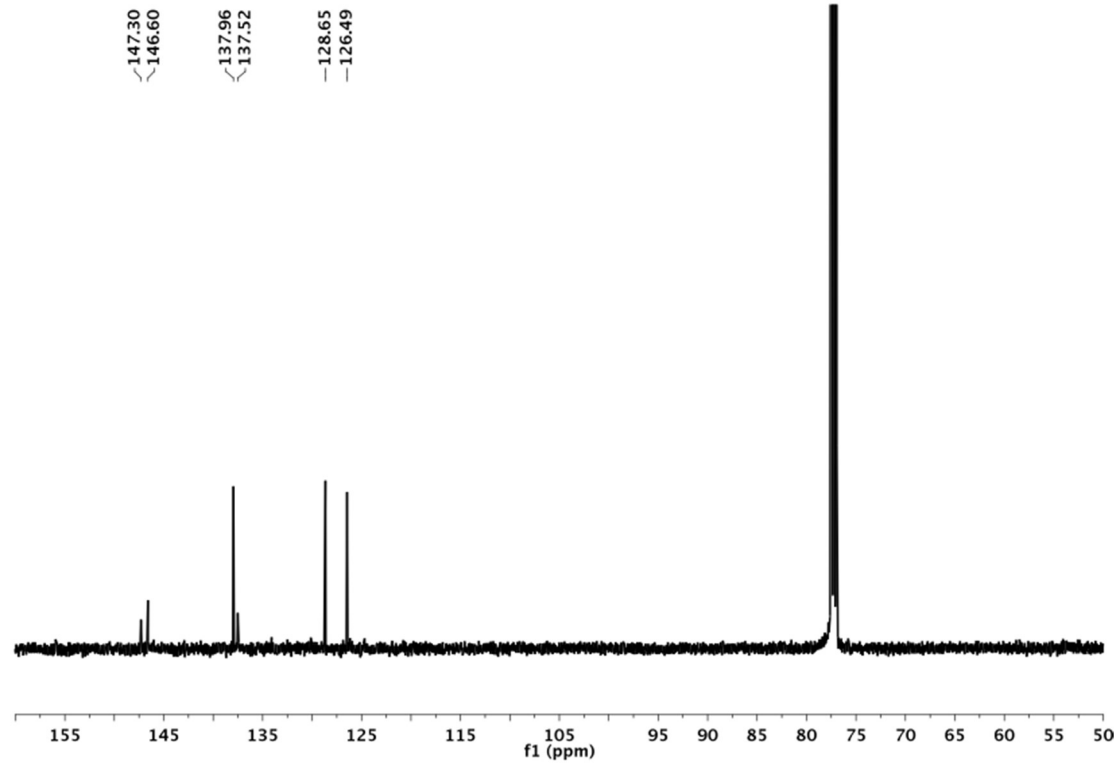


Figure S3. ^{13}C (dept135) NMR spectrum of **1** in $CDCl_3$ at room temperature.

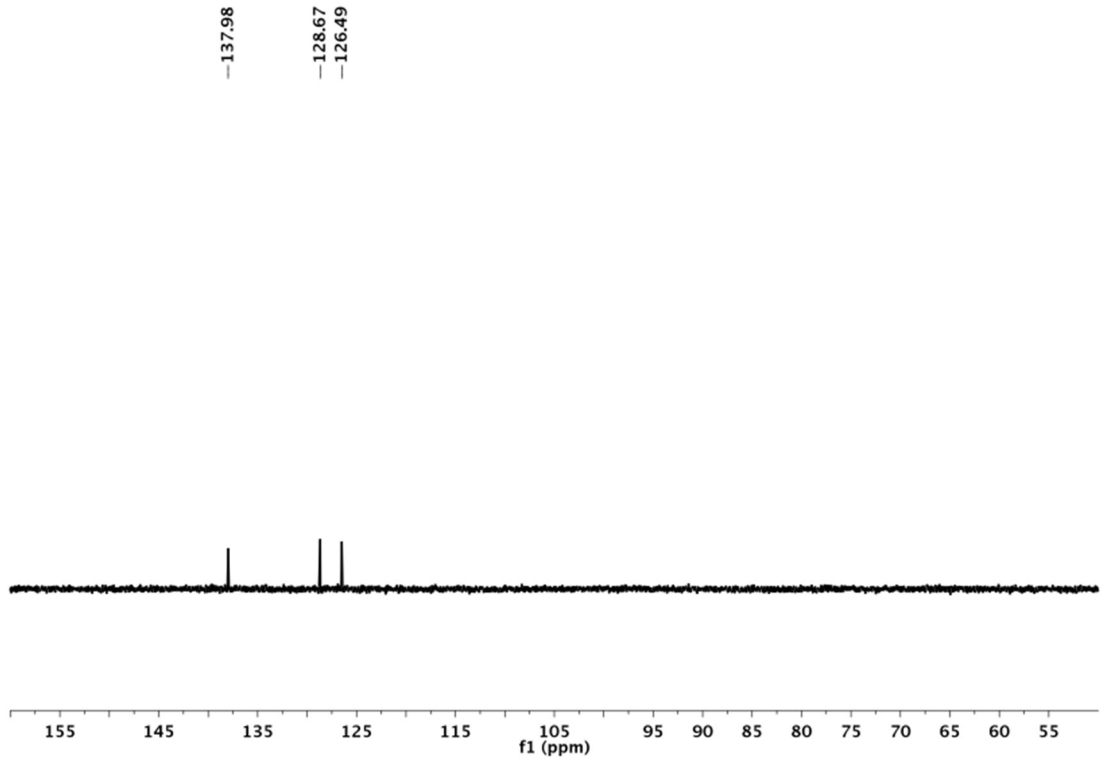


Figure S4. ATR-IR spectrum of **1**.

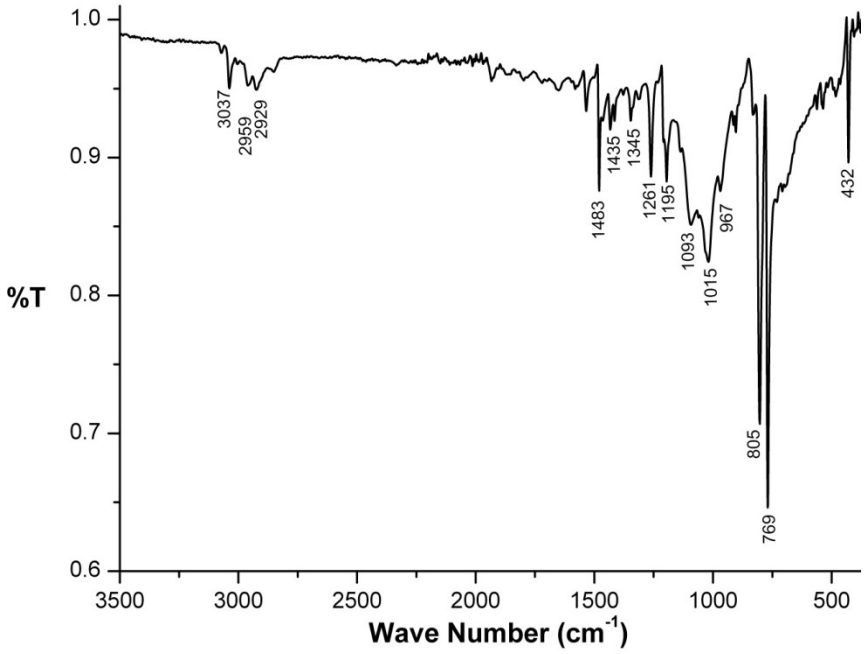


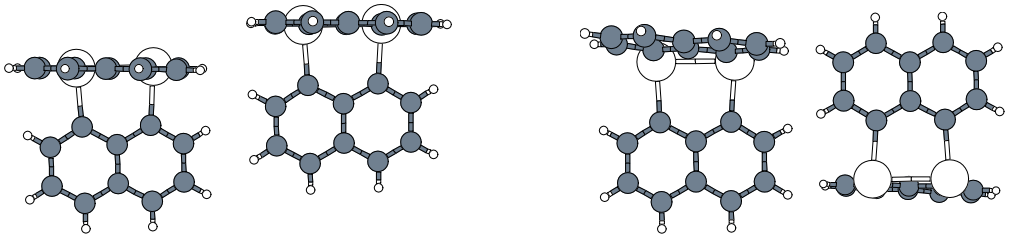
Table S1: Crystallographic details of 1

Identification code	**1**
Empirical formula	C_{20} H_{12} Sb_2
M	495.80
Crystal size [mm]	0.256 × 0.184 × 0.072
T [K]	100(1)
Crystal system	triclinic
Space group	P -1
a [Å]	8.4505(6)
b [Å]	9.0047(6)
c [Å]	11.1040(7)
α [°]	75.645(2)
β [°]	69.497(3)
γ [°]	86.077(3)
V [Å^3]	766.56(9)
Z	2
D_{calc} [g · cm^{-1}]	2.148
μ(MoK_α [mm^{-1}])	3.516
Transmissions	0.75/0.60
F(000)	468
Index ranges	$-13 \leq h \leq 12$
	$-13 \leq k \leq 13$
	$-17 \leq l \leq 16$
θ_{max} [°]	33.225
Reflections collected	26589
Independent reflections	5779
R_{int}	0.0214
Refined parameters	199
R_1 [$I > 2\sigma(I)$]	0.0228
wR_2 [all data]	0.0536
GooF	1.083
$\Delta\rho_{final}$ (max/min) [e · Å^{-3}]	3.958/-1.824

Quantum chemical calculation

The structures of **1a'**, **1b'** and **1c'** and the free monomer **1** were fully optimized using tightened convergence criteria and improved integration grids at the density functional theory level (DFT) in the resolution-of-the-identity approximation (RI), employing the BP exchange-correlation functional[1] and a third-generation dispersion correction[2] as implemented in the Turbomole quantum chemistry program package.[3] A triple-zeta (TZ) quality Gaussian type function basis set termed def2-TZVP[4] has been used along with the appropriate auxiliary RI basis set,[5] in conjunction with an effective core potential for Sb.[6] Atom coordinates and energies of the optimized geometries are given below. The BP+D3/def2-TZVP level of theory was also used to calculate interaction energies for the crystal structure dimer motifs **1a**, **1b**, **1c**, **1d** and **1e** (for the latter see figure S6) and the corresponding fragment-fragment interaction energies in **1a-1c**, without counterpoise correction.[7] Completely analogous geometry optimization and interaction analyzation were carried out for the structural motifs 1b'(E) and 1c'(E) resulting from the replacement from Sb with the pnictogen atoms E= P, As, and Bi. Furthermore geometry optimizations were also carried out with PBE+D3/def2-TZVP [2,8], and fragment-fragment interaction energies on the BP+D3 optimized structures were additionally calculated with PBE+D3/def2-TZVP.

Figure S5. (left **1d**, right **1e**)



On the other hand, fragment-fragment interaction energies were determined with density-fitting DFT-SAPT[9] with the asymptotically corrected[10] PBE0 exchange-correlation (xc) potential (PBE0AC)[11] and the adiabatic local density approximation (ALDA) for the exchange-correlation kernel[12] using the Molpro implementation.[13] The orbital basis set in the DFT-SAPT calculations was chosen to be aug-cc-pVTZ[14], complemented by the corresponding aug-cc-pVTZ MP2[15] and JK[16] density fitting

auxiliary basis sets. However, for technical reasons def2-TZVPP[4] orbital and def2-ATZVPP MP2[17] and JK[18] auxiliary basis sets were used for the Sb atom, again with an effective core potential.[6] The ionization potentials and highest occupied molecular orbital energies needed for the asymptotic correction were extracted from Kohn-Sham calculations (unrestricted for the cation) with the PBE0 xc functional. The total SAPT interaction energy then was calculated as

$$E_{int} = E_{el}^{(1)} + E_{exc}^{(1)} + E_{ind}^{(2)} + E_{ind-exch}^{(2)} + E_{disp}^{(2)} + E_{disp-exch}^{(2)} + \delta(\mathrm{HF}),$$

where $E_{el}^{(1)}$ is the first-order electrostatic interaction energy, $E_{exch}^{(1)}$ the first-order exchange contribution, $E_{ind}^{(2)}$ and $E_{ind-exch}^{(2)}$ the second-order induction energy and its accompanying exchange- correction, $E_{disp}^{(2)}$ and $E_{disp-exch}^{(2)}$ the second-order dispersion and exchange-dispersion contributions, and δ(HF) an estimate of higher-order induction and exchange-induction contributions[19] as determined from the difference of supermolecular counterpoise-corrected[7] Hartree-Fock and Hartree-Fock level SAPT calculations of the sum of $E_{el}^{(1)}$ + $E_{exch}^{(1)}$ + $E_{ind}^{(2)}$ + $E_{ind-exch}^{(2)}$ with the aug-cc-pVTZ/def2-TZVPP (Sb) basis set. For the purpose of analysis it is convenient to group some of the above contributions to the total induction energy

$$E_{IND} = E_{ind}^{(2)} + E_{ind}^{(2)} + E_{ind-exch}^{(2)} + \delta(\mathrm{HF})$$

and to the total dispersion energy

$$E_{DISP} = E_{disp}^{(2)} + E_{disp-exch}^{(2)}.$$

In addition fragment-fragment interaction energies were determined with counterpoise-corrected spin-component- scaled second order Møller-Plesset perturbation theory (SCS-MP2),[20] using the aug-cc-pVTZ orbital basis set along with the corresponding MP2 auxiliary RI basis set in the Turbomole implementation.

For the purpose of comparison with coupled cluster theory at the CCSD(T) level the DFT-SAPT calculations were repeated with smaller aug-cc-pVDZ /def2-SVP (Sb) combinations of basis sets and effective core potentials, reducing the auxiliary basis sets accordingly to aug-cc-pVDZ MP2 and JK fitting for C and H and to def2-ASVP MP2 and JK fitting for Sb. SCS-MP2 calculations were additionally carried out with aug-cc-pVDZ. Finally, DFT-SAPT and SCS-MP2 interaction energies were determined for the fragments containing the other pnictogen atoms as well, with analogous double- and triple-zeta basis sets.

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1’(Sb) optimized at the BP+D3/def2-TZVP level of theory: Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1250.523777948

Sb	-1.4034699	2.5330025	0.1710508
Sb	1.3319075	2.5349314	-0.4647003
C	-0.8825417	1.1443911	1.7758589
C	-1.9056998	0.6827515	2.5861727
H	-2.9288866	1.0345695	2.4338630
C	-1.6578478	-0.2529052	3.6184523
H	-2.4837156	-0.6058368	4.2380939
C	-0.3771416	-0.7095257	3.8371156
H	-0.1731197	-1.4285744	4.6334948
C	0.7065947	-0.2520828	3.0412912
C	0.4597191	0.6986486	1.9811719
C	1.5730801	1.1443066	1.2038010
C	2.8488200	0.6818744	1.4781337
H	3.6994283	1.0335271	0.8893313
C	3.0824407	-0.2544053	2.5131681
H	4.0969364	-0.6081784	2.7034286
C	2.0302527	-0.7104255	3.2756873
H	2.1989667	-1.4297259	4.0800582
C	-1.6027221	0.9528948	-1.3253808
C	-2.8644252	0.4258893	-1.5419834
H	-3.7254901	0.8189573	-0.9961464
C	-3.0698733	-0.6299249	-2.4615024
H	-4.0736615	-1.0318834	-2.6077939
C	-2.0040553	-1.1410096	-3.1681653
H	-2.1512108	-1.9528514	-3.8837879
C	-0.6942537	-0.6214010	-2.9907099
C	-0.4759908	0.4521484	-2.0480437
C	0.8527893	0.9566079	-1.8980970
C	1.8898327	0.4334345	-2.6513389
H	2.9024471	0.8291866	-2.5424178
C	1.6701527	-0.6220193	-3.5680321
H	2.5066886	-1.0208652	-4.1439613
C	0.4032217	-1.1368858	-3.7302580
H	0.2208270	-1.9486208	-4.4378543

1a'(Sb) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2501.085164698

Sb	-1.9980544	4.0317041	-1.6446141
Sb	0.7418408	4.0549089	-2.2606582
C	-1.4815900	2.6690134	-0.0219542
C	-2.4960267	2.2454221	0.8204232
H	-3.5114309	2.6291982	0.6941453
C	-2.2480456	1.3037578	1.8464706
H	-3.0658769	0.9740181	2.4891262
C	-0.9819613	0.7913428	2.0185904

H	-0.7843996	0.0480776	2.7913712
C	0.0894982	1.2098967	1.1882685
C	-0.1502787	2.1803787	0.1458604
C	0.9596984	2.5934327	-0.6538183
C	2.2196473	2.0658624	-0.4309606
H	3.0660751	2.3868754	-1.0431150
C	2.4379921	1.0924863	0.5720228
H	3.4314365	0.6640738	0.7098151
C	1.3934597	0.6796450	1.3651180
H	1.5512859	-0.0721718	2.1359658
C	-2.1584164	2.4275549	-3.1262861
C	-3.3945509	1.8250946	-3.2907106
H	-4.2572572	2.1789808	-2.7211972
C	-3.5688920	0.7350714	-4.1760253
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H	-2.6246636	-0.5696036	-5.5984861
C	-1.2196210	0.8701947	-4.7947617
C	-1.0297089	1.9697109	-3.8757981
C	0.2811712	2.5259704	-3.7520428
C	1.3216520	2.0426840	-4.5275447
H	2.3209989	2.4745782	-4.4355691
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C	-0.1180982	0.3958409	-5.5558913
H	-0.2776678	-0.4391134	-6.2411649
Sb	1.9980991	-4.0317167	1.6445764
Sb	-0.7417935	-4.0549740	2.2606198
C	1.4816499	-2.6689732	0.0219619
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C	2.2481032	-1.3037029	-1.8464534
H	3.0659109	-0.9740426	-2.4891812
C	0.9820275	-0.7912557	-2.0185403
H	0.7844687	-0.0479907	-2.7913326
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C	-1.3933932	-0.6795755	-1.3650466
H	-1.5512320	0.0722260	-2.1359026
C	2.1584065	-2.4276262	3.1263184
C	3.3945310	-1.8251541	3.2907703
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C	3.5688605	-0.7351805	4.1761479
H	4.5498124	-0.2672455	4.2712387
C	2.5014170	-0.2704949	4.9119908

H	2.6245963	0.5694637	5.5986120
C	1.2195390	-0.8702262	4.7947201
C	1.0296946	-1.9698499	3.8758696
C	-0.2811789	-2.5261231	3.7521117
C	-1.3216424	-2.0429488	4.5277030
H	-2.3209871	-2.4748391	4.4356907
C	-1.1263945	-0.9731012	5.4338407
H	-1.9662690	-0.6040365	6.0243607
C	0.1179385	-0.3956948	5.5556216
H	0.2775443	0.4391233	6.2410528

1b'(Sb) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2501.072099841

Sb	-2.4431598	-0.4119478	-1.9812206
Sb	0.2908305	-0.3684502	-2.6122507
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C	-2.9024687	-2.1250337	0.5447540
H	-3.9268873	-1.7744593	0.3981372
C	-2.6386524	-3.0243394	1.6050202
H	-3.4526648	-3.3460210	2.2564489
C	-1.3582836	-3.4878252	1.8096562
H	-1.1425794	-4.1807959	2.6255749
C	-0.2879729	-3.0635313	0.9780130
C	-0.5497921	-2.1405987	-0.1036079
C	0.5525580	-1.7074471	-0.9039863
C	1.8320631	-2.1620888	-0.6332369
H	2.6755069	-1.8148346	-1.2346240
C	2.0791145	-3.0803193	0.4156042
H	3.0970508	-3.4249232	0.6028388
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C	-2.9250747	-4.3098898	-5.0869719
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C	-0.1437646	-2.0315575	-3.9675096
C	0.9055607	-2.5528173	-4.7052007
H	1.9027958	-2.1124417	-4.6280971
C	0.7200234	-3.6632881	-5.5627856
H	1.5661930	-4.0581722	-6.1275005
C	-0.5259915	-4.2379790	-5.6810778
H	-0.6817236	-5.0941081	-6.3412726
Sb	2.4415519	0.4110958	1.9770958

Sb	-0.2912880	0.3691452	2.6130467
C	1.8908239	1.7029645	0.3035396
C	2.8978348	2.1314242	-0.5444242
H	3.9228177	1.7822162	-0.3984946
C	2.6325002	3.0318384	-1.6033512
H	3.4459846	3.3558604	-2.2542803
C	1.3512800	3.4931674	-1.8075432
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C	0.5452067	2.1422488	0.1041239
C	-0.5563621	1.7063535	0.9040559
C	-1.8367912	2.1583695	0.6333457
H	-2.6796355	1.8086926	1.2341555
C	-2.0855744	3.0769441	-0.4148002
H	-3.1042280	3.4194115	-0.6020576
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H	-1.2272584	4.2179760	-2.0203784
C	2.5933714	2.0941124	3.3690918
C	3.8361520	2.6795236	3.5421884
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C	4.0107709	3.7927749	4.3981814
H	5.0000895	4.2395732	4.5097660
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H	3.0575127	5.1584152	5.7564310
C	1.6427922	3.7260076	4.9556858
C	1.4563832	2.5949223	4.0757373
C	0.1462545	2.0341202	3.9652087
C	-0.9024654	2.5593952	4.7009200
H	-1.9009899	2.1221315	4.6227765
C	-0.7145667	3.6697887	5.5580598
H	-1.5603245	4.0679418	6.1210942
C	0.5333213	4.2399908	5.6784357
H	0.6910055	5.0956528	6.3387709

1c' (Sb) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2501.074055646

Sb	-0.2253440	0.9216462	3.4416553
Sb	2.5145308	0.8605497	2.8435372
C	0.2340553	-0.5421677	5.0012046
C	-0.8162926	-1.0130304	5.7707205
H	-1.8291590	-0.6371918	5.6063649
C	-0.6110057	-1.9887756	6.7748208
H	-1.4582851	-2.3482203	7.3610399
C	0.6557998	-2.4755304	7.0095136
H	0.8273323	-3.2245992	7.7857046
C	1.7666590	-2.0109709	6.2564459
C	1.5622565	-1.0217448	5.2229387
C	2.7008759	-0.5726653	4.4847255

C	3.9614090	-1.0663814	4.7746358
H	4.8315217	-0.7133981	4.2156760
C	4.1543934	-2.0376664	5.7856811
H	5.1579086	-2.4150199	5.9888468
C	3.0764198	-2.4996579	6.5075813
H	3.2133633	-3.2474032	7.2918752
C	-0.4495533	-0.6029048	1.8970000
C	-1.7243536	-1.0711905	1.6366495
H	-2.5852280	-0.6346842	2.1470746
C	-1.9444037	-2.1157508	0.7081906
H	-2.9592060	-2.4724286	0.5257131
C	-0.8798612	-2.6707980	0.0333296
H	-1.0382666	-3.4784209	-0.6847673
C	0.4435307	-2.1991064	0.2453767
C	0.6763528	-1.1404718	1.2000922
C	2.0160297	-0.6836912	1.3838112
C	3.0500352	-1.2282212	0.6415118
H	4.0709994	-0.8612934	0.7711711
C	2.8160625	-2.2653546	-0.2901582
H	3.6493114	-2.6824634	-0.8577932
C	1.5378356	-2.7449012	-0.4758415
H	1.3450238	-3.5477257	-1.1905295
Sb	0.2254171	-0.9219054	-3.4412365
Sb	-2.5147922	-0.8608790	-2.8446732
C	-0.2330525	0.5418009	-5.0011218
C	0.8176625	1.0123356	-5.7703278
H	1.8303348	0.6360608	-5.6057892
C	0.6130117	1.9883445	-6.7743050
H	1.4605698	2.3475241	-7.3602802
C	-0.6535243	2.4757181	-7.0091570
H	-0.8245522	3.2250413	-7.7852129
C	-1.7647551	2.0114902	-6.2564296
C	-1.5610121	1.0219464	-5.2230924
C	-2.7000080	0.5731314	-4.4853073
C	-3.9602634	1.0674625	-4.7753917
H	-4.8306707	0.7146843	-4.2167588
C	-4.1525866	2.0391023	-5.7862183
H	-5.1558922	2.4169406	-5.9895272
C	-3.0742425	2.5008038	-6.5077563
H	-3.2106807	3.2487818	-7.2919165
C	0.4486360	0.6029290	-1.8967166
C	1.7231603	1.0720401	-1.6365043
H	2.5843288	0.6361498	-2.1469425
C	1.9425681	2.1167902	-0.7081033
H	2.9570985	2.4744323	-0.5260065
C	0.8777454	2.6710204	-0.0330070
H	1.0357069	3.4786916	0.6851348
C	-0.4453532	2.1985121	-0.2449668
C	-0.6775763	1.1398637	-1.1998494
C	-2.0170452	0.6826299	-1.3839365

C -3.0514135 1.2266220 -0.6417492
H -4.0722327 0.8593937 -0.7717546
C -2.8180171 2.2636134 0.2902374
H -3.6515547 2.6802716 0.8577765
C -1.5400156 2.7436468 0.4762209
H -1.3477472 3.5466435 1.1908705

1'(Sb) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1249.206237161
Sb -1.4026546 2.5037504 0.1726644
Sb 1.3319630 2.5056770 -0.4629100
C -0.8796088 1.1273586 1.7854387
C -1.9007082 0.6757909 2.6038406
H -2.9247975 1.0249228 2.4473124
C -1.6501808 -0.2448300 3.6481324
H -2.4750736 -0.5909526 4.2738219
C -0.3684611 -0.6953537 3.8716331
H -0.1605398 -1.4029912 4.6779091
C 0.7131307 -0.2459268 3.0693155
C 0.4633528 0.6884883 1.9966352
C 1.5747592 1.1273323 1.2137237
C 2.8522280 0.6750061 1.4963176
H 3.7018139 1.0240211 0.9034057
C 3.0887280 -0.2462332 2.5433414
H 4.1050168 -0.5932273 2.7394759
C 2.0377476 -0.6961724 3.3106075
H 2.2073423 -1.4039597 4.1256733
C -1.6038579 0.9348196 -1.3332501
C -2.8675744 0.4168628 -1.5592007
H -3.7275375 0.8078638 -1.0089935
C -3.0763481 -0.6254725 -2.4923672
H -4.0821277 -1.0213688 -2.6453205
C -2.0119039 -1.1311056 -3.2044385
H -2.1602287 -1.9328917 -3.9318908
C -0.7009361 -0.6186597 -3.0192836
C -0.4792787 0.4402020 -2.0622415
C 0.8503925 0.9385036 -1.9056126
C 1.8850749 0.4243413 -2.6681045
H 2.8986597 0.8179596 -2.5547452
C 1.6622684 -0.6176021 -3.5985159
H 2.4975981 -1.0103048 -4.1813855
C 0.3941635 -1.1270287 -3.7661951
H 0.2075780 -1.9288194 -4.4847934

1a'(Sb) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2498.439562141
Sb -1.9843616 4.0504340 -1.6830949

Sb	0.7387182	4.1314018	-2.3592151
C	-1.3988582	2.6947287	-0.0785784
C	-2.3944966	2.2103513	0.7525657
H	-3.4309874	2.5279937	0.6099545
C	-2.1004528	1.2917297	1.7866357
H	-2.9044382	0.9079309	2.4176453
C	-0.8037748	0.8780011	1.9895172
H	-0.5671337	0.1647271	2.7806125
C	0.2510523	1.3642880	1.1743083
C	-0.0407080	2.2952112	0.1098276
C	1.0467298	2.7638706	-0.6885983
C	2.3399206	2.3430097	-0.4292134
H	3.1697711	2.7132129	-1.0373530
C	2.6145887	1.4227929	0.6087413
H	3.6395069	1.0893214	0.7824637
C	1.5890007	0.9443984	1.3916555
H	1.7895506	0.2300757	2.1916557
C	-2.1611753	2.4686351	-3.1827517
C	-3.4087188	1.9002204	-3.3776853
H	-4.2709490	2.2646704	-2.8130525
C	-3.5968800	0.8367764	-4.2917303
H	-4.5890631	0.3989269	-4.4161258
C	-2.5285706	0.3590359	-5.0176222
H	-2.6600271	-0.4628595	-5.7252224
C	-1.2341773	0.9225057	-4.8654367
C	-1.0337026	2.0035128	-3.9277709
C	0.2824555	2.5437711	-3.7919164
C	1.3233005	2.0460863	-4.5576628
H	2.3269298	2.4678748	-4.4580933
C	1.1219334	0.9824754	-5.4687785
H	1.9632994	0.6013198	-6.0505452
C	-0.1322652	0.4331017	-5.6154630
H	-0.3007431	-0.3898327	-6.3139721
Sb	1.9843640	-4.0504316	1.6830771
Sb	-0.7387091	-4.1314074	2.3592221
C	1.3988447	-2.6947227	0.0785693
C	2.3944751	-2.2103393	-0.7525806
H	3.4309693	-2.5279714	-0.6099729
C	2.1004194	-1.2917172	-1.7866466
H	2.9043960	-0.9079260	-2.4176718
C	0.8037388	-0.8779904	-1.9895146
H	0.5670885	-0.1647140	-2.7806045
C	-0.2510802	-1.3642848	-1.1743004
C	0.0406917	-2.2952097	-0.1098245
C	-1.0467383	-2.7638758	0.6886088
C	-2.3399326	-2.3430182	0.4292345
H	-3.1697727	-2.7131974	1.0374032
C	-2.6146129	-1.4228029	-0.6087186
H	-3.6395332	-1.0893323	-0.7824303
C	-1.5890322	-0.9444014	-1.3916383

H	-1.7895911	-0.2300777	-2.1916355
C	2.1611894	-2.4686357	3.1827354
C	3.4087339	-1.9002204	3.3776600
H	4.2709598	-2.2646680	2.8130195
C	3.5969013	-0.8367787	4.2917061
H	4.5890859	-0.3989316	4.4160978
C	2.5285971	-0.3590383	5.0176056
H	2.6600570	0.4628615	5.7251998
C	1.2342033	-0.9225097	4.8654303
C	1.0337223	-2.0035159	3.9277645
C	-0.2824364	-2.5437760	3.7919198
C	-1.3232758	-2.0460920	4.5576745
H	-2.3269059	-2.4678807	4.4581122
C	-1.1219026	-0.9824825	5.4687905
H	-1.9632643	-0.6013289	6.0505651
C	0.1322967	-0.4331081	5.6154663
H	0.3007794	0.3898251	6.3139755

1b'(Sb) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2498.428720104

Sb	-2.4822215	-0.4914011	-2.0489592
Sb	0.2507154	-0.4409100	-2.6857968
C	-1.9219215	-1.7547072	-0.3575418
C	-2.9262859	-2.1768323	0.4964691
H	-3.9558153	-1.8453010	0.3371367
C	-2.6527638	-3.0465083	1.5781152
H	-3.4649617	-3.3677425	2.2329686
C	-1.3654606	-3.4809508	1.8001148
H	-1.1401899	-4.1502323	2.6338410
C	-0.2991107	-3.0580205	0.9635362
C	-0.5714954	-2.1688837	-0.1422659
C	0.5263470	-1.7417949	-0.9511205
C	1.8123085	-2.1661500	-0.6627839
H	2.6521316	-1.8213045	-1.2718334
C	2.0704767	-3.0488577	0.4126605
H	3.0936832	-3.3715929	0.6134342
C	1.0330922	-3.4848817	1.2061097
H	1.2204426	-4.1581834	2.0459750
C	-2.6296661	-2.1709848	-3.4418028
C	-3.8727409	-2.7531322	-3.6226084
H	-4.7436823	-2.3629295	-3.0890197
C	-4.0466007	-3.8592113	-4.4870391
H	-5.0366444	-4.3041130	-4.6045672
C	-2.9685059	-4.3649148	-5.1785306
H	-3.0903591	-5.2153218	-5.8539260
C	-1.6778968	-3.7902932	-5.0383427
C	-1.4921256	-2.6669153	-4.1498005
C	-0.1823194	-2.1080436	-4.0333746

C	0.8667555	-2.6278051	-4.7723142
H	1.8651133	-2.1895780	-4.6901246
C	0.6795520	-3.7314671	-5.6372553
H	1.5261275	-4.1259469	-6.2026222
C	-0.5683758	-4.2996092	-5.7631941
H	-0.7273046	-5.1503935	-6.4303706
Sb	2.4837662	0.4917697	2.0481689
Sb	-0.2488415	0.4395011	2.6861966
C	1.9219293	1.7549532	0.3571077
C	2.9257482	2.1782609	-0.4969721
H	3.9555439	1.8472759	-0.3382348
C	2.6513283	3.0485730	-1.5778706
H	3.4631050	3.3707318	-2.2327931
C	1.3637121	3.4825262	-1.7990405
H	1.1377560	4.1523000	-2.6321868
C	0.2979091	3.0584034	-0.9623816
C	0.5711952	2.1685050	0.1425961
C	-0.5261143	1.7400313	0.9514444
C	-1.8125099	2.1633791	0.6635422
H	-2.6519570	1.8170226	1.2722427
C	-2.0715415	3.0469933	-0.4109543
H	-3.0950420	3.3690833	-0.6112660
C	-1.0346345	3.4846659	-1.2041128
H	-1.2226655	4.1587126	-2.0432300
C	2.6307483	2.1715292	3.4408405
C	3.8735336	2.7544498	3.6211289
H	4.7445129	2.3647359	3.0872462
C	4.0470363	3.8607114	4.4853990
H	5.0368592	4.3062016	4.6025549
C	2.9688809	4.3658432	5.1772126
H	3.0904568	5.2164089	5.8524581
C	1.6785695	3.7904248	5.0375487
C	1.4931605	2.6668362	4.1491975
C	0.1836466	2.1071830	4.0332655
C	-0.8654854	2.6264022	4.7725065
H	-1.8636178	2.1875940	4.6906770
C	-0.6786443	3.7302733	5.6372572
H	-1.5252595	4.1243077	6.2028753
C	0.5689884	4.2991733	5.7627054
H	0.7276294	5.1501514	6.4297034

1c'(Sb) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2498.430446354

Sb	-0.1829864	0.8132779	3.4706106
Sb	2.5591330	0.7443241	2.8853392
C	0.2726336	-0.6096601	5.0660739
C	-0.7783640	-1.0575180	5.8481459
H	-1.7917028	-0.6883466	5.6686077

C	-0.5732957	-1.9987153	6.8839240
H	-1.4215518	-2.3412300	7.4797491
C	0.6941439	-2.4731861	7.1378500
H	0.8671967	-3.1957669	7.9391448
C	1.8052795	-2.0300369	6.3733857
C	1.6011089	-1.0769062	5.3076009
C	2.7403256	-0.6481538	4.5594048
C	4.0015893	-1.1265053	4.8706750
H	4.8724583	-0.7864386	4.3038628
C	4.1942628	-2.0632310	5.9130746
H	5.1989205	-2.4296782	6.1326697
C	3.1152596	-2.5052281	6.6453215
H	3.2506916	-3.2262177	7.4552477
C	-0.4026187	-0.7219918	1.9359655
C	-1.6790513	-1.1792157	1.6614727
H	-2.5397775	-0.7476608	2.1781677
C	-1.9012940	-2.2015648	0.7096817
H	-2.9179916	-2.5477852	0.5141063
C	-0.8363740	-2.7490141	0.0291344
H	-0.9955993	-3.5389271	-0.7091186
C	0.4889651	-2.2943433	0.2618212
C	0.7232816	-1.2549093	1.2365689
C	2.0646458	-0.8083072	1.4338739
C	3.1001771	-1.3526906	0.6939483
H	4.1232502	-0.9946706	0.8366555
C	2.8652575	-2.3755694	-0.2532611
H	3.7004323	-2.7927416	-0.8191473
C	1.5841050	-2.8370494	-0.4601869
H	1.3883432	-3.6232702	-1.1932266
Sb	0.1857458	-0.8117877	-3.4705168
Sb	-2.5569142	-0.7458129	-2.8874052
C	-0.2700552	0.6114401	-5.0657115
C	0.7811169	1.0607475	-5.8467127
H	1.7947189	0.6926820	-5.6663968
C	0.5758847	2.0020716	-6.8823434
H	1.4242591	2.3456991	-7.4773588
C	-0.6918696	2.4752006	-7.1372052
H	-0.8650421	3.1978509	-7.9384120
C	-1.8031713	2.0305187	-6.3738760
C	-1.5988553	1.0772128	-5.3082750
C	-2.7382496	0.6468341	-4.5612884
C	-3.9997704	1.1239358	-4.8734343
H	-4.8707472	0.7827066	-4.3074857
C	-4.1925898	2.0608539	-5.9156355
H	-5.1974640	2.4262748	-6.1359493
C	-3.1134472	2.5043455	-6.6467721
H	-3.2489790	3.2255221	-7.4565154
C	0.4026127	0.7228949	-1.9348718
C	1.6783866	1.1810331	-1.6588876
H	2.5400269	0.7504210	-2.1748494

C	1.8988558	2.2032191	-0.7064792
H	2.9150845	2.5502113	-0.5098413
C	0.8327917	2.7495135	-0.0268020
H	0.9905960	3.5392413	0.7119573
C	-0.4919445	2.2938712	-0.2610412
C	-0.7244445	1.2546519	-1.2364376
C	-2.0652573	0.8071113	-1.4353234
C	-3.1019387	1.3502300	-0.6960714
H	-4.1245707	0.9913879	-0.8398937
C	-2.8687816	2.3729194	0.2517864
H	-3.7048769	2.7891765	0.8170016
C	-1.5882189	2.8354021	0.4601159
H	-1.3937458	3.6213479	1.1937880

1'(P) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1452.5513647770

P	-1.1296056	2.1465029	0.1347740
P	1.0743282	2.1456341	-0.3778379
C	-0.8923881	1.0428605	1.5997298
C	-1.9303935	0.6504420	2.4274671
H	-2.9492484	0.9906994	2.2329701
C	-1.6791977	-0.2035493	3.5284256
H	-2.5103122	-0.5112254	4.1647997
C	-0.3990640	-0.6398560	3.8086674
H	-0.2125710	-1.2904693	4.6654594
C	0.6962491	-0.2416037	2.9965534
C	0.4358092	0.6113137	1.8751624
C	1.5059162	1.0379993	1.0390766
C	2.8018672	0.6414598	1.3216761
H	3.6301196	0.9780108	0.6952424
C	3.0617284	-0.2116890	2.4213271
H	4.0876913	-0.5227533	2.6238059
C	2.0368566	-0.6432366	3.2403925
H	2.2471324	-1.2924856	4.0927304
C	-1.5306693	0.8739052	-1.1466198
C	-2.8154942	0.4145711	-1.3807273
H	-3.6533221	0.7990684	-0.7960153
C	-3.0512898	-0.5646386	-2.3758147
H	-4.0683665	-0.9239057	-2.5396719
C	-2.0142188	-1.0596932	-3.1419073
H	-2.2061846	-1.8069531	-3.9145396
C	-0.6850940	-0.5974654	-2.9478212
C	-0.4484133	0.3830818	-1.9302708
C	0.8676636	0.8780197	-1.7082873
C	1.9159837	0.4242506	-2.4904126
H	2.9249153	0.8126238	-2.3390024
C	1.6884917	-0.5547176	-3.4876180
H	2.5277851	-0.9091369	-4.0879153
C	0.4208763	-1.0546250	-3.7131188

H	0.2524195	-1.8024393	-4.4906797

1a'(P) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2905.1382827390

P	-3.4241839	0.3917658	2.6816575
P	-3.7163054	1.9992023	1.1137997
C	-3.9314249	-0.9638447	1.5287579
C	-3.9727648	-2.2972211	1.9003451
C	-4.3264339	-3.2901782	0.9547215
C	-4.6562523	-2.9485995	-0.3425320
C	-4.6527335	-1.5893632	-0.7560466
C	-4.9850556	-1.1719855	-2.0728401
C	-4.9659168	0.1668972	-2.4124178
C	-4.6096849	1.1531873	-1.4607114
C	-4.2531034	0.7842213	-0.1744799
C	-4.2835743	-0.5888074	0.2011603
C	-1.5956000	0.3257814	2.4180042
C	-0.7564058	-0.5094874	3.1349798
C	0.6326265	-0.5239565	2.8631714
C	1.1765223	0.3060222	1.9044851
C	0.3516250	1.1933490	1.1655931
C	0.8541445	2.0747052	0.1734645
C	0.0048443	2.9214006	-0.5087521
C	-1.3838187	2.9346660	-0.2351690
C	-1.9138063	2.0725622	0.7091646
C	-1.0557071	1.1955733	1.4298264
H	-3.7157016	-2.5925934	2.9192237
H	-4.3362477	-4.3375556	1.2597136
H	-4.9279874	-3.7204855	-1.0649231
H	-5.2604593	-1.9256868	-2.8128592
H	-5.2269659	0.4737534	-3.4262127
H	-4.6012213	2.2046345	-1.7537733
H	-1.1619089	-1.1716279	3.9024810
H	1.2796843	-1.2051381	3.4174988
H	2.2467260	0.2867535	1.7021228
H	1.9212507	2.0720102	-0.0449148
H	0.4065725	3.5875466	-1.2735145
H	-2.0342985	3.6182896	-0.7842332
P	3.4241839	-0.3917658	-2.6816575
P	3.7163054	-1.9992023	-1.1137997
C	3.9314249	0.9638447	-1.5287579
C	3.9727648	2.2972211	-1.9003451
C	4.3264339	3.2901782	-0.9547215
C	4.6562523	2.9485995	0.3425320
C	4.6527335	1.5893632	0.7560466
C	4.9850556	1.1719855	2.0728401
C	4.9659168	-0.1668972	2.4124178
C	4.6096849	-1.1531873	1.4607114

C	4.2531034	-0.7842213	0.1744799
C	4.2835743	0.5888074	-0.2011603
C	1.5956000	-0.3257814	-2.4180042
C	0.7564058	0.5094874	-3.1349798
C	-0.6326265	0.5239565	-2.8631714
C	-1.1765223	-0.3060222	-1.9044851
C	-0.3516250	-1.1933490	-1.1655931
C	-0.8541445	-2.0747052	-0.1734645
C	-0.0048443	-2.9214006	0.5087521
C	1.3838187	-2.9346660	0.2351690
C	1.9138063	-2.0725622	-0.7091646
C	1.0557071	-1.1955733	-1.4298264
H	3.7157016	2.5925934	-2.9192237
H	4.3362477	4.3375556	-1.2597136
H	4.9279874	3.7204855	1.0649231
H	5.2604593	1.9256868	2.8128592
H	5.2269659	-0.4737534	3.4262127
H	4.6012213	-2.2046345	1.7537733
H	1.1619089	1.1716279	-3.9024810
H	-1.2796843	1.2051381	-3.4174988
H	-2.2467260	-0.2867535	-1.7021228
H	-1.9212507	-2.0720102	0.0449148
H	-0.4065725	-3.5875466	1.2735145
H	2.0342985	-3.6182896	0.7842332

1b'(P) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2905.1238581970

P	-1.8264983	-0.4986367	-1.8519212
P	0.3648551	-0.6031974	-2.4009119
C	-1.5964813	-1.5139242	-0.3246209
C	-2.6253563	-1.8029898	0.5545537
H	-3.6285233	-1.4121666	0.3742098
C	-2.3851883	-2.6141369	1.6893971
H	-3.2086200	-2.8360512	2.3697548
C	-1.1246032	-3.1129457	1.9498499
H	-0.9453632	-3.7267822	2.8345775
C	-0.0360359	-2.8184990	1.0864064
C	-0.2846979	-2.0020080	-0.0646146
C	0.7805673	-1.6681555	-0.9475436
C	2.0607839	-2.1243820	-0.6848774
H	2.8874273	-1.8505621	-1.3429837
C	2.3063311	-2.9482556	0.4388670
H	3.3206401	-3.3017795	0.6287354
C	1.2863719	-3.2869179	1.3057585
H	1.4889282	-3.9056740	2.1820061
C	-2.2883105	-1.8481903	-3.0320725
C	-3.5882639	-2.2945289	-3.1997997
H	-4.3995441	-1.8603340	-2.6122328

C	-3.8743123	-3.3243535	-4.1282759
H	-4.9027939	-3.6716096	-4.2390935
C	-2.8724267	-3.8835885	-4.8975331
H	-3.1034853	-4.6698111	-5.6191507
C	-1.5292131	-3.4393690	-4.7705727
C	-1.2420887	-2.4085052	-3.8177253
C	0.0898488	-1.9324491	-3.6585437
C	1.1050456	-2.4528998	-4.4428910
H	2.1265238	-2.0819228	-4.3385356
C	0.8277937	-3.4786122	-5.3789563
H	1.6417590	-3.8848410	-5.9814862
C	-0.4558770	-3.9621430	-5.5406454
H	-0.6624348	-4.7479547	-6.2701527
P	1.8182725	0.4949476	1.8579643
P	-0.3745965	0.6081720	2.3987167
C	1.5978146	1.5099002	0.3290069
C	2.6310935	1.7945816	-0.5464409
H	3.6321217	1.4002130	-0.3619705
C	2.3982441	2.6058898	-1.6826939
H	3.2251291	2.8245127	-2.3599305
C	1.1404600	3.1090420	-1.9483590
H	0.9668176	3.7228516	-2.8342139
C	0.0474814	2.8187216	-1.0891521
C	0.2888224	2.0024124	0.0635514
C	-0.7810838	1.6727853	0.9424942
C	-2.0588193	2.1325393	0.6740066
H	-2.8890296	1.8619435	1.3289472
C	-2.2972481	2.9558828	-0.4516857
H	-3.3097222	3.3121171	-0.6461956
C	-1.2726628	3.2906886	-1.3145941
H	-1.4697173	3.9091271	-2.1923241
C	2.2809606	1.8435428	3.0388185
C	3.5820215	2.2848236	3.2112517
H	4.3938515	1.8468816	2.6272344
C	3.8685450	3.3143164	4.1399531
H	4.8979649	3.6575559	4.2545093
C	2.8658863	3.8782683	4.9047460
H	3.0972708	4.6641379	5.6266440
C	1.5213938	3.4393874	4.7728253
C	1.2339004	2.4087706	3.8198231
C	-0.0992745	1.9378014	3.6558948
C	-1.1154496	2.4630516	4.4357690
H	-2.1379727	2.0960040	4.3278065
C	-0.8378051	3.4885935	5.3719001
H	-1.6525101	3.8986533	5.9708247
C	0.4471362	3.9671727	5.5381784
H	0.6539458	4.7528878	6.2677179

1c'(P) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2905.1298965770

P	2.5598852	0.4361995	2.6244227
P	2.2912465	2.0415733	1.0554003
C	2.0660070	-0.9178021	1.4679990
C	1.9635143	-2.2426266	1.8548485
C	1.5552392	-3.2267279	0.9224182
C	1.2408015	-2.8838950	-0.3778246
C	1.3173985	-1.5326047	-0.8073570
C	0.9718486	-1.1115994	-2.1191619
C	1.0211279	0.2250654	-2.4645036
C	1.4170716	1.2048127	-1.5241702
C	1.7827850	0.8299850	-0.2434507
C	1.7341414	-0.5404147	0.1370112
C	4.3957400	0.3825826	2.4018529
C	5.2250649	-0.4436133	3.1410554
C	6.6230461	-0.4348738	2.9170427
C	7.1847172	0.4085006	1.9784368
C	6.3705691	1.2868730	1.2145536
C	6.8874637	2.1872440	0.2450031
C	6.0445467	3.0269895	-0.4564370
C	4.6477240	3.0120587	-0.2255503
C	4.1033253	2.1340851	0.6961044
C	4.9550545	1.2653742	1.4352893
H	2.1940986	-2.5363439	2.8807364
H	1.4814897	-4.2671224	1.2428993
H	0.9043622	-3.6432901	-1.0852417
H	0.6429224	-1.8571860	-2.8451535
H	0.7246583	0.5362843	-3.4667437
H	1.4116824	2.2572457	-1.8105830
H	4.8061161	-1.1123100	3.8954703
H	7.2606642	-1.1004609	3.5009324
H	8.2648036	0.4157585	1.8183361
H	7.9645903	2.2116959	0.0676352
H	6.4553382	3.7175654	-1.1945563
H	4.0030593	3.6919205	-0.7859277
P	-2.5598852	-0.4361995	-2.6244227
P	-2.2912465	-2.0415733	-1.0554003
C	-2.0660070	0.9178021	-1.4679990
C	-1.9635143	2.2426266	-1.8548485
C	-1.5552392	3.2267279	-0.9224182
C	-1.2408015	2.8838950	0.3778246
C	-1.3173985	1.5326047	0.8073570
C	-0.9718486	1.1115994	2.1191619
C	-1.0211279	-0.2250654	2.4645036
C	-1.4170716	-1.2048127	1.5241702
C	-1.7827850	-0.8299850	0.2434507
C	-1.7341414	0.5404147	-0.1370112
C	-4.3957400	-0.3825826	-2.4018529
C	-5.2250649	0.4436133	-3.1410554
C	-6.6230461	0.4348738	-2.9170427

C	-7.1847172	-0.4085006	-1.9784368
C	-6.3705691	-1.2868730	-1.2145536
C	-6.8874637	-2.1872440	-0.2450031
C	-6.0445467	-3.0269895	0.4564370
C	-4.6477240	-3.0120587	0.2255503
C	-4.1033253	-2.1340851	-0.6961044
C	-4.9550545	-1.2653742	-1.4352893
H	-2.1940986	2.5363439	-2.8807364
H	-1.4814897	4.2671224	-1.2428993
H	-0.9043622	3.6432901	1.0852417
H	-0.6429224	1.8571860	2.8451535
H	-0.7246583	-0.5362843	3.4667437
H	-1.4116824	-2.2572457	1.8105830
H	-4.8061161	1.1123100	-3.8954703
H	-7.2606642	1.1004609	-3.5009324
H	-8.2648036	-0.4157585	-1.8183361
H	-7.9645903	-2.2116959	-0.0676352
H	-6.4553382	-3.7175654	1.1945563
H	-4.0030593	-3.6919205	0.7859277

1'(P) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1451.1279989630

P	-1.1276523	2.1165908	0.1371814
P	1.0700777	2.1181849	-0.3730628
C	-0.8915158	1.0200085	1.6058367
C	-1.9276090	0.6364691	2.4399357
H	-2.9473818	0.9744491	2.2433000
C	-1.6736399	-0.2027090	3.5507596
H	-2.5039460	-0.5049116	4.1917044
C	-0.3924653	-0.6318742	3.8354571
H	-0.2029747	-1.2704042	4.7013424
C	0.7010291	-0.2400869	3.0187369
C	0.4375962	0.5968566	1.8865656
C	1.5063771	1.0208505	1.0485290
C	2.8044399	0.6384890	1.3404270
H	3.6326595	0.9772403	0.7141919
C	3.0669917	-0.2006662	2.4492825
H	4.0950791	-0.5019414	2.6585340
C	2.0429582	-0.6307167	3.2696387
H	2.2551175	-1.2692353	4.1302825
C	-1.5317751	0.8561123	-1.1524742
C	-2.8184348	0.4080688	-1.3976637
H	-3.6565099	0.7914174	-0.8115412
C	-3.0563815	-0.5560103	-2.4059608
H	-4.0755355	-0.9068658	-2.5784467
C	-2.0199068	-1.0460733	-3.1754545
H	-2.2133755	-1.7817158	-3.9595581
C	-0.6895882	-0.5931588	-2.9719981
C	-0.4506480	0.3710551	-1.9400657

C	0.8659153	0.8593221	-1.7106201
C	1.9130412	0.4149738	-2.4995747
H	2.9228134	0.8008314	-2.3435838
C	1.6835299	-0.5485677	-3.5103162
H	2.5224519	-0.8964626	-4.1158892
C	0.4151062	-1.0421356	-3.7429060
H	0.2441561	-1.7773845	-4.5325896

1a'(P) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2902.282013524

P	-1.7213613	3.7000310	-1.7344468
P	0.4736060	3.7419506	-2.2574528
C	-1.4521893	2.6456227	-0.2424610
C	-2.4720483	2.2679499	0.6139719
H	-3.4977510	2.5936204	0.4268521
C	-2.1930630	1.4455343	1.7311162
H	-3.0101412	1.1384763	2.3867586
C	-0.9054479	1.0279229	2.0005383
H	-0.7005309	0.3937834	2.8647142
C	0.1707284	1.4168530	1.1606343
C	-0.1155128	2.2378800	0.0229970
C	0.9381371	2.6571353	-0.8359556
C	2.2416610	2.2793635	-0.5636447
H	3.0578969	2.6106082	-1.2095922
C	2.5234872	1.4492134	0.5467821
H	3.5527000	1.1389724	0.7365030
C	1.5165091	1.0297123	1.3918344
H	1.7456220	0.3953148	2.2491375
C	-2.0997057	2.3957199	-2.9901707
C	-3.3704707	1.8855055	-3.1960480
H	-4.2109147	2.2438455	-2.5977173
C	-3.5878689	0.8857564	-4.1740978
H	-4.5932373	0.4835046	-4.3115204
C	-2.5484679	0.4210329	-4.9561022
H	-2.7257891	-0.3460008	-5.7131364
C	-1.2351127	0.9365561	-4.7938523
C	-1.0162206	1.9355393	-3.7901883
C	0.2866916	2.4707827	-3.5865505
C	1.3373887	2.0438533	-4.3808505
H	2.3366085	2.4625777	-4.2433266
C	1.1274118	1.0504907	-5.3674142
H	1.9700375	0.7152159	-5.9749158
C	-0.1258814	0.5067071	-5.5699934
H	-0.2802551	-0.2572648	-6.3351339
P	1.7213420	-3.7000854	1.7344578
P	-0.4736875	-3.7419522	2.2574356
C	1.4521905	-2.6456252	0.2425011
C	2.4720868	-2.2678473	-0.6138405

H	3.4978643	-2.5931078	-0.4264201
C	2.1930979	-1.4455786	-1.7310913
H	3.0101262	-1.1388765	-2.3869619
C	0.9054971	-1.0279225	-2.0005097
H	0.7005963	-0.3937722	-2.8646819
C	-0.1706986	-1.4168546	-1.1606300
C	0.1155141	-2.2378897	-0.0229908
C	-0.9381628	-2.6571334	0.8359367
C	-2.2416713	-2.2793091	0.5636257
H	-3.0579022	-2.6104025	1.2096574
C	-2.5234741	-1.4491971	-0.5468341
H	-3.5526981	-1.1390525	-0.7366527
C	-1.5164709	-1.0296920	-1.3918526
H	-1.7455517	-0.3953020	-2.2491683
C	2.0996924	-2.3958103	2.9902043
C	3.3704277	-1.8854595	3.1959507
H	4.2108692	-2.2438017	2.5976183
C	3.5878344	-0.8857273	4.1740106
H	4.5931607	-0.4833192	4.3112809
C	2.5484667	-0.4211172	4.9561208
H	2.7258400	0.3457395	5.7133224
C	1.2351045	-0.9366219	4.7938649
C	1.0161914	-1.9355762	3.7901766
C	-0.2867399	-2.4707761	3.5865185
C	-1.3374266	-2.0438286	4.3808202
H	-2.3366582	-2.4625215	4.2432851
C	-1.1274080	-1.0505440	5.3674536
H	-1.9700269	-0.7152554	5.9749572
C	0.1258891	-0.5067695	5.5700242
H	0.2802693	0.2572228	6.3351429

1c'(P) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2902.2743447700

P	2.6701504	0.3952299	2.6088881
P	2.3949362	1.9946045	1.0434578
C	2.1803524	-0.9622409	1.4566943
C	2.0837662	-2.2873045	1.8445894
C	1.6703379	-3.2722162	0.9161344
C	1.3389329	-2.9291189	-0.3796180
C	1.4068805	-1.5779452	-0.8097059
C	1.0455111	-1.1575903	-2.1170680
C	1.0939526	0.1780574	-2.4651913
C	1.5034140	1.1575021	-1.5304475
C	1.8840852	0.7836754	-0.2535537
C	1.8359584	-0.5857037	0.1289929
C	4.5066056	0.3636181	2.4038907
C	5.3406518	-0.4456463	3.1562020
C	6.7403586	-0.4130642	2.9501371

C	7.2989915	0.4384808	2.0176804
C	6.4800162	1.3017103	1.2428314
C	6.9939040	2.2120432	0.2818669
C	6.1464560	3.0391443	-0.4283460
C	4.7479389	3.0004771	-0.2153960
C	4.2063141	2.1101411	0.6958485
C	5.0626580	1.2550828	1.4443471
H	2.3242249	-2.5802668	2.8690459
H	1.6043472	-4.3136428	1.2368465
H	0.9966667	-3.6898079	-1.0841556
H	0.7057354	-1.9044195	-2.8377940
H	0.7896409	0.4891317	-3.4659442
H	1.5007352	2.2103515	-1.8190699
H	4.9234123	-1.1185235	3.9086110
H	7.3822307	-1.0663399	3.5441489
H	8.3813280	0.4654669	1.8717865
H	8.0733539	2.2553095	0.1195538
H	6.5553847	3.7391884	-1.1593397
H	4.0989879	3.6732867	-0.7803379
P	-2.6701504	-0.3952299	-2.6088881
P	-2.3949362	-1.9946045	-1.0434578
C	-2.1803524	0.9622409	-1.4566943
C	-2.0837662	2.2873045	-1.8445894
C	-1.6703379	3.2722162	-0.9161344
C	-1.3389329	2.9291189	0.3796180
C	-1.4068805	1.5779452	0.8097059
C	-1.0455111	1.1575903	2.1170680
C	-1.0939526	-0.1780574	2.4651913
C	-1.5034140	-1.1575021	1.5304475
C	-1.8840852	-0.7836754	0.2535537
C	-1.8359584	0.5857037	-0.1289929
C	-4.5066056	-0.3636181	-2.4038907
C	-5.3406518	0.4456463	-3.1562020
C	-6.7403586	0.4130642	-2.9501371
C	-7.2989915	-0.4384808	-2.0176804
C	-6.4800162	-1.3017103	-1.2428314
C	-6.9939040	-2.2120432	-0.2818669
C	-6.1464560	-3.0391443	0.4283460
C	-4.7479389	-3.0004771	0.2153960
C	-4.2063141	-2.1101411	-0.6958485
C	-5.0626580	-1.2550828	-1.4443471
H	-2.3242249	2.5802668	-2.8690459
H	-1.6043472	4.3136428	-1.2368465
H	-0.9966667	3.6898079	1.0841556
H	-0.7057354	1.9044195	2.8377940
H	-0.7896409	-0.4891317	3.4659442
H	-1.5007352	-2.2103515	1.8190699
H	-4.9234123	1.1185235	-3.9086110
H	-7.3822307	1.0663399	-3.5441489
H	-8.3813280	-0.4654669	-1.8717865

H	-8.0733539	-2.2553095	-0.1195538
H	-6.5553847	-3.7391884	1.1593397
H	-4.0989879	-3.6732867	0.7803379

1'(As) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -5242.0725376120

As	-1.2354201	2.3292756	0.1453228
As	1.1699631	2.3306523	-0.4144200
C	-0.8925022	1.0941455	1.6593806
C	-1.9252812	0.6687316	2.4742783
H	-2.9453332	1.0165153	2.2980526
C	-1.6757146	-0.2285304	3.5407180
H	-2.5046528	-0.5596692	4.1681457
C	-0.3956851	-0.6776246	3.7904670
H	-0.2018356	-1.3646834	4.6167890
C	0.6949068	-0.2499497	2.9871831
C	0.4410984	0.6547496	1.8981092
C	1.5315451	1.0931477	1.0936374
C	2.8179514	0.6662582	1.3668975
H	3.6549161	1.0132620	0.7572892
C	3.0654753	-0.2315336	2.4333704
H	4.0861426	-0.5640723	2.6285646
C	2.0279458	-0.6793816	3.2242263
H	2.2192968	-1.3665290	4.0510652
C	-1.5598754	0.9172185	-1.2101241
C	-2.8333812	0.4259171	-1.4303456
H	-3.6807292	0.8173883	-0.8635261
C	-3.0538926	-0.5955128	-2.3857297
H	-4.0645738	-0.9765712	-2.5398635
C	-2.0028882	-1.1026122	-3.1211013
H	-2.1735773	-1.8857639	-3.8627012
C	-0.6827878	-0.6115740	-2.9373451
C	-0.4562313	0.4195631	-1.9603925
C	0.8641790	0.9206302	-1.7759733
C	1.9098259	0.4330749	-2.5379715
H	2.9194793	0.8272438	-2.4046443
C	1.6872360	-0.5878941	-3.4933808
H	2.5261631	-0.9658556	-4.0797261
C	0.4206977	-1.0984517	-3.6875845
H	0.2475389	-1.8815644	-4.4286669

1a'(As) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -10484.1816536900

As	-1.8326388	3.8384242	-1.6802657
As	0.5780448	3.8535608	-2.2192450
C	-1.4946249	2.6376844	-0.1410379
C	-2.5210485	2.2541695	0.7028574

H	-3.5342834	2.6296431	0.5440459
C	-2.2728164	1.3608885	1.7725163
H	-3.0960115	1.0561323	2.4205067
C	-1.0051477	0.8642743	1.9903435
H	-0.8168028	0.1637228	2.8042687
C	0.0756603	1.2485070	1.1551937
C	-0.1705782	2.1611084	0.0722634
C	0.9184635	2.5620143	-0.7532754
C	2.1903648	2.0741211	-0.5193016
H	3.0246282	2.3846153	-1.1521370
C	2.4231166	1.1520871	0.5291774
H	3.4247433	0.7491902	0.6832223
C	1.3913459	0.7544222	1.3499982
H	1.5706719	0.0448873	2.1552114
C	-2.1239199	2.3952064	-3.0142625
C	-3.3746712	1.8304327	-3.1869900
H	-4.2229566	2.1818746	-2.5959455
C	-3.5678180	0.7787034	-4.1149115
H	-4.5580234	0.3337556	-4.2229735
C	-2.5156474	0.3180439	-4.8791757
H	-2.6654317	-0.4912257	-5.5963879
C	-1.2201074	0.8851946	-4.7479325
C	-1.0185943	1.9396434	-3.7900528
C	0.2864537	2.4867563	-3.6262054
C	1.3348486	2.0382045	-4.4086769
H	2.3327007	2.4649270	-4.2884665
C	1.1336010	1.0061793	-5.3576962
H	1.9752429	0.6566190	-5.9574024
C	-0.1130387	0.4378471	-5.5178516
H	-0.2662658	-0.3649628	-6.2416130
As	1.8326404	-3.8384340	1.6802828
As	-0.5780173	-3.8535884	2.2192447
C	1.4946532	-2.6377029	0.1410422
C	2.5210800	-2.2541756	-0.7028498
H	3.5343180	-2.6296451	-0.5440353
C	2.2728464	-1.3608936	-1.7725094
H	3.0960447	-1.0561170	-2.4204868
C	1.0051722	-0.8643015	-1.9903561
H	0.8168319	-0.1637560	-2.8042856
C	-0.0756383	-1.2485340	-1.1552086
C	0.1706036	-2.1611266	-0.0722696
C	-0.9184346	-2.5620286	0.7532811
C	-2.1903309	-2.0741115	0.5193212
H	-3.0245975	-2.3846104	1.1521508
C	-2.4230814	-1.1520771	-0.5291573
H	-3.4246913	-0.7491270	-0.6831593
C	-1.3913241	-0.7544555	-1.3500128
H	-1.5706518	-0.0449385	-2.1552371
C	2.1239120	-2.3952102	3.0142803
C	3.3746595	-1.8304229	3.1870192

H	4.2229371	-2.1818306	2.5959395
C	3.5677927	-0.7786899	4.1149393
H	4.5579981	-0.3337452	4.2230203
C	2.5156103	-0.3180299	4.8791875
H	2.6653735	0.4912678	5.5963715
C	1.2200760	-0.8851934	4.7479394
C	1.0185851	-1.9396708	3.7900867
C	-0.2864612	-2.4867940	3.6262253
C	-1.3348653	-2.0382460	4.4086879
H	-2.3327208	-2.4649531	4.2884489
C	-1.1336593	-1.0061232	5.3576098
H	-1.9753130	-0.6565446	5.9572882
C	0.1129879	-0.4378245	5.5178181
H	0.2662047	0.3649819	6.2415842

1b'(As) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -10484.1713933700

As	-2.1449677	-0.4284096	-1.8758384
As	0.2612376	-0.4290758	-2.4320972
C	-1.7907718	-1.5609012	-0.2880503
C	-2.8097266	-1.9083951	0.5788962
H	-3.8224883	-1.5344012	0.4147602
C	-2.5566404	-2.7620825	1.6797416
H	-3.3743825	-3.0279090	2.3513203
C	-1.2882209	-3.2527182	1.9064537
H	-1.0920589	-3.9074469	2.7578092
C	-0.2089875	-2.8994567	1.0535275
C	-0.4640945	-2.0268196	-0.0613570
C	0.6195144	-1.6355052	-0.8983427
C	1.8998728	-2.0879437	-0.6382821
H	2.7337078	-1.7666873	-1.2655698
C	2.1458448	-2.9664129	0.4440242
H	3.1627960	-3.3132037	0.6317341
C	1.1158497	-3.3613388	1.2716242
H	1.3093925	-4.0222715	2.1187667
C	-2.4411641	-1.9425728	-3.1285079
C	-3.7009653	-2.4882514	-3.2947936
H	-4.5493397	-2.0966752	-2.7292431
C	-3.9065275	-3.5641916	-4.1917119
H	-4.9062780	-3.9873821	-4.3018188
C	-2.8555263	-4.0707528	-4.9280248
H	-3.0156697	-4.8948633	-5.6264407
C	-1.5497476	-3.5271956	-4.7990977
C	-1.3380953	-2.4436923	-3.8770456
C	-0.0312424	-1.8942006	-3.7402496
C	1.0141021	-2.3818165	-4.5026294
H	2.0133226	-1.9516295	-4.4058501
C	0.8061203	-3.4505320	-5.4082122

H	1.6450467	-3.8270762	-5.9956874
C	-0.4459376	-4.0115120	-5.5509103
H	-0.6072282	-4.8336959	-6.2513624
As	2.1450012	0.4284131	1.8758287
As	-0.2612402	0.4290731	2.4321051
C	1.7907883	1.5609053	0.2880445
C	2.8097379	1.9084071	-0.5789049
H	3.8224857	1.5343533	-0.4148194
C	2.5566516	2.7621252	-1.6797262
H	3.3744275	3.0280993	-2.3512053
C	1.2882165	3.2527055	-1.9064696
H	1.0920186	3.9073105	-2.7579119
C	0.2089915	2.8994568	-1.0535278
C	0.4641057	2.0268227	0.0613603
C	-0.6195046	1.6355045	0.8983479
C	-1.8998647	2.0879393	0.6382826
H	-2.7337024	1.7666782	1.2655644
C	-2.1458392	2.9664021	-0.4440281
H	-3.1627912	3.3131913	-0.6317372
C	-1.1158477	3.3613271	-1.2716311
H	-1.3093953	4.0222462	-2.1187832
C	2.4411631	1.9425733	3.1285117
C	3.7009599	2.4882635	3.2947931
H	4.5493333	2.0967019	2.7292312
C	3.9065193	3.5641983	4.1917180
H	4.9062741	3.9873728	4.3018476
C	2.8555130	4.0707659	4.9280186
H	3.0156467	4.8948989	5.6264102
C	1.5497398	3.5271929	4.7991041
C	1.3380929	2.4436798	3.8770612
C	0.0312379	1.8941905	3.7402649
C	-1.0141060	2.3818022	4.5026486
H	-2.0133299	1.9516262	4.4058568
C	-0.8061213	3.4505068	5.4082431
H	-1.6450303	3.8269970	5.9957780
C	0.4459244	4.0115241	5.5508992
H	0.6071970	4.8337641	6.2512895

1c'(As) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -10484.1743169600

As	0.0300519	0.7764100	3.2432732
As	2.4492187	0.6627976	2.7734558
C	0.2538401	-0.5008292	4.7459541
C	-0.8302395	-0.8911867	5.5104176
H	-1.8251404	-0.4938427	5.2984407
C	-0.6671775	-1.8164831	6.5696117
H	-1.5361280	-2.1191824	7.1559707
C	0.5792727	-2.3289807	6.8637895
H	0.7063250	-3.0380038	7.6845187

C	1.7208055	-1.9402078	6.1132655
C	1.5543264	-1.0074845	5.0309763
C	2.6953581	-0.6096073	4.2768067
C	3.9480004	-1.1018295	4.5938390
H	4.8241459	-0.7873745	4.0227404
C	4.1100356	-2.0260736	5.6542240
H	5.1051958	-2.4100886	5.8837894
C	3.0215871	-2.4360797	6.3957483
H	3.1469745	-3.1446735	7.2171329
C	-0.3147990	-0.5944198	1.8554080
C	-1.6032813	-1.0033751	1.5705132
H	-2.4513874	-0.5571470	2.0920671
C	-1.8394063	-1.9905148	0.5847578
H	-2.8631319	-2.2973541	0.3670346
C	-0.7888471	-2.5454518	-0.1162259
H	-0.9739414	-3.2973277	-0.8859034
C	0.5479258	-2.1343234	0.1325635
C	0.7903693	-1.1405124	1.1426678
C	2.1255572	-0.7120302	1.3840806
C	3.1709318	-1.2276124	0.6408357
H	4.1924097	-0.8824088	0.8142216
C	2.9308469	-2.2059659	-0.3532630
H	3.7681152	-2.6032355	-0.9291270
C	1.6491335	-2.6525603	-0.5986957
H	1.4607333	-3.3967977	-1.3743622
As	-0.0300540	-0.7764116	-3.2432745
As	-2.4492200	-0.6627967	-2.7734576
C	-0.2538409	0.5008291	-4.7459548
C	0.8302389	0.8911861	-5.5104184
H	1.8251395	0.4938401	-5.2984425
C	0.6671779	1.8164838	-6.5696116
H	1.5361291	2.1191843	-7.1559690
C	-0.5792720	2.3289817	-6.8637900
H	-0.7063240	3.0380037	-7.6845202
C	-1.7208050	1.9402102	-6.1132655
C	-1.5543265	1.0074869	-5.0309763
C	-2.6953584	0.6096100	-4.2768071
C	-3.9480002	1.1018339	-4.5938385
H	-4.8241461	0.7873776	-4.0227415
C	-4.1100345	2.0260795	-5.6542223
H	-5.1051936	2.4100996	-5.8837839
C	-3.0215864	2.4360824	-6.3957487
H	-3.1469740	3.1446730	-7.2171360
C	0.3147978	0.5944178	-1.8554089
C	1.6032803	1.0033728	-1.5705139
H	2.4513864	0.5571435	-2.0920676
C	1.8394056	1.9905135	-0.5847594
H	2.8631314	2.2973529	-0.3670368
C	0.7888466	2.5454517	0.1162236
H	0.9739412	3.2973288	0.8858996

C	-0.5479262	2.1343228	-0.1325649
C	-0.7903701	1.1405112	-1.1426682
C	-2.1255580	0.7120292	-1.3840805
C	-3.1709315	1.2276094	-0.6408330
H	-4.1924060	0.8823899	-0.8142018
C	-2.9308469	2.2059664	0.3532621
H	-3.7681151	2.6032367	0.9291255
C	-1.6491335	2.6525598	0.5986946
H	-1.4607327	3.3967970	1.3743609

1'(As) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -5239.7994969460

As	-1.2326817	2.3000083	0.1463367
As	1.1681077	2.3013235	-0.4121891
C	-0.8900636	1.0758208	1.6664915
C	-1.9209395	0.6604356	2.4888310
H	-2.9418166	1.0057244	2.3090322
C	-1.6689456	-0.2209761	3.5670572
H	-2.4970641	-0.5450005	4.2001647
C	-0.3879275	-0.6632275	3.8222033
H	-0.1908992	-1.3379097	4.6586344
C	0.7007826	-0.2438802	3.0130001
C	0.4441153	0.6436994	1.9112972
C	1.5325876	1.0752503	1.1016213
C	2.8206368	0.6589653	1.3830367
H	3.6569231	1.0038250	0.7702780
C	3.0710660	-0.2228692	2.4612896
H	4.0935687	-0.5478338	2.6624649
C	2.0348352	-0.6643808	3.2568681
H	2.2277084	-1.3391038	4.0942443
C	-1.5603418	0.8984423	-1.2160136
C	-2.8357977	0.4167461	-1.4455450
H	-3.6823735	0.8065245	-0.8753310
C	-3.0596950	-0.5903141	-2.4144175
H	-4.0724224	-0.9645681	-2.5753323
C	-2.0101878	-1.0917500	-3.1552134
H	-2.1827595	-1.8638297	-3.9087033
C	-0.6888107	-0.6088392	-2.9636478
C	-0.4588787	0.4068679	-1.9722299
C	0.8623174	0.9013715	-1.7809583
C	1.9057835	0.4227493	-2.5514515
H	2.9163520	0.8148151	-2.4143047
C	1.6802754	-0.5839123	-3.5203756
H	2.5181735	-0.9555745	-4.1131594
C	0.4125408	-1.0882709	-3.7207066
H	0.2358312	-1.8603288	-4.4732721

1a'(As) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -10479.62555525

As	-1.8168247	3.8593688	-1.7137375
As	0.5762960	3.9233637	-2.3019680
C	-1.4219612	2.6637703	-0.1858021
C	-2.4299571	2.2289733	0.6546814
H	-3.4623135	2.5447535	0.4855062
C	-2.1385669	1.3608197	1.7333459
H	-2.9478381	1.0104352	2.3768388
C	-0.8439497	0.9529479	1.9726968
H	-0.6210359	0.2813527	2.8032161
C	0.2204545	1.3955041	1.1448924
C	-0.0737796	2.2685492	0.0415565
C	0.9926171	2.7178943	-0.7870498
C	2.2936899	2.3312818	-0.5239636
H	3.1120973	2.6878203	-1.1542050
C	2.5781865	1.4598702	0.5538854
H	3.6077790	1.1463674	0.7364438
C	1.5656691	1.0031697	1.3697055
H	1.7863611	0.3306326	2.1998391
C	-2.1197693	2.4327189	-3.0580168
C	-3.3801689	1.8989511	-3.2558821
H	-4.2290425	2.2633372	-2.6725427
C	-3.5846345	0.8675589	-4.2037052
H	-4.5844469	0.4498622	-4.3355716
C	-2.5317093	0.3928267	-4.9577775
H	-2.6886126	-0.4018950	-5.6905045
C	-1.2261184	0.9287591	-4.8000507
C	-1.0157935	1.9691018	-3.8291514
C	0.2923397	2.5060426	-3.6595682
C	1.3402078	2.0454610	-4.4357620
H	2.3409134	2.4666686	-4.3139529
C	1.1344163	1.0158988	-5.3853843
H	1.9769715	0.6567387	-5.9791938
C	-0.1194540	0.4689646	-5.5621053
H	-0.2794956	-0.3252578	-6.2947197
As	1.8168245	-3.8593609	1.7137271
As	-0.5762878	-3.9233524	2.3019871
C	1.4219317	-2.6637632	0.1857968
C	2.4299164	-2.2289668	-0.6547012
H	3.4622763	-2.5447395	-0.4855327
C	2.1385112	-1.3608245	-1.7333703
H	2.9477731	-1.0104484	-2.3768794
C	0.8438893	-0.9529619	-1.9727120
H	0.6209601	-0.2813836	-2.8032412
C	-0.2205046	-1.3955148	-1.1448934
C	0.0737457	-2.2685475	-0.0415529
C	-0.9926387	-2.7178915	0.7870700
C	-2.2937164	-2.3312875	0.5239936

H	-3.1121167	-2.6878350	1.1542393
C	-2.5782292	-1.4598844	-0.5538577
H	-3.6078255	-1.1463883	-0.7364058
C	-1.5657236	-1.0031872	-1.3696940
H	-1.7864283	-0.3306581	-2.1998314
C	2.1197910	-2.4327103	3.0580005
C	3.3801935	-1.8989389	3.2558429
H	4.2290582	-2.2633282	2.6724922
C	3.5846770	-0.8675582	4.2036736
H	4.5844921	-0.4498642	4.3355272
C	2.5317640	-0.3928307	4.9577659
H	2.6886785	0.4018897	5.6904920
C	1.2261690	-0.9287587	4.8000549
C	1.0158267	-1.9690910	3.8291510
C	-0.2923102	-2.5060279	3.6595809
C	-1.3401666	-2.0454441	4.4357899
H	-2.3408760	-2.4666449	4.3139889
C	-1.1343597	-1.0158858	5.3854126
H	-1.9769082	-0.6567190	5.9792275
C	0.1195156	-0.4689604	5.5621234
H	0.2795702	0.3252560	6.2947415

1c'(As) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -10479.6181873100

As	0.0597118	0.6804699	3.2883705
As	2.4753766	0.5683155	2.8206546
C	0.2864226	-0.5705150	4.8095447
C	-0.7948579	-0.9477135	5.5843603
H	-1.7919466	-0.5590380	5.3638575
C	-0.6265184	-1.8461387	6.6648369
H	-1.4940001	-2.1396712	7.2589788
C	0.6228531	-2.3433233	6.9711427
H	0.7553247	-3.0311414	7.8096040
C	1.7616433	-1.9652234	6.2121341
C	1.5893732	-1.0614156	5.1071653
C	2.7277021	-0.6733044	4.3451098
C	3.9839348	-1.1456338	4.6774476
H	4.8588035	-0.8351839	4.1011427
C	4.1517647	-2.0418829	5.7599242
H	5.1503176	-2.4111013	6.0012978
C	3.0654235	-2.4430483	6.5087316
H	3.1944275	-3.1300628	7.3484177
C	-0.2843992	-0.6914265	1.9031438
C	-1.5736663	-1.0917351	1.6079405
H	-2.4220255	-0.6485879	2.1337562
C	-1.8109142	-2.0666255	0.6105219
H	-2.8358205	-2.3674146	0.3861980
C	-0.7596558	-2.6191597	-0.0910457

H	-0.9439351	-3.3621358	-0.8703977
C	0.5778761	-2.2195424	0.1701494
C	0.8206028	-1.2355062	1.1894650
C	2.1562681	-0.8136920	1.4392762
C	3.2029700	-1.3328288	0.7003881
H	4.2256816	-0.9931414	0.8811055
C	2.9637771	-2.3073028	-0.2973900
H	3.8031146	-2.7092725	-0.8680655
C	1.6805087	-2.7413566	-0.5557872
H	1.4918680	-3.4806217	-1.3372100
As	-0.0596950	-0.6803718	-3.2882635
As	-2.4753724	-0.5682433	-2.8207807
C	-0.2862934	0.5703701	-4.8096302
C	0.7949821	0.9471774	-5.5846437
H	1.7920115	0.5583456	-5.3641513
C	0.6267126	1.8453740	-6.6653212
H	1.4941901	2.1385685	-7.2596355
C	-0.6225791	2.3427859	-6.9715800
H	-0.7549934	3.0304602	-7.8101684
C	-1.7613652	1.9651067	-6.2123544
C	-1.5891844	1.0614306	-5.1072633
C	-2.7275293	0.6736362	-4.3450765
C	-3.9836671	1.1463429	-4.6772370
H	-4.8585508	0.8361835	-4.1007978
C	-4.1513918	2.0425437	-5.7597684
H	-5.1498595	2.4121030	-6.0009751
C	-3.0650529	2.4432614	-6.5088217
H	-3.1939838	3.1302218	-7.3485637
C	0.2842583	0.6916632	-1.9031164
C	1.5734809	1.0920858	-1.6078538
H	2.4219164	0.6490722	-2.1336672
C	1.8106403	2.0669884	-0.6104226
H	2.8354930	2.3681130	-0.3863306
C	0.7592831	2.6194604	0.0910677
H	0.9434582	3.3626033	0.8702875
C	-0.5781736	2.2195763	-0.1700355
C	-0.8207953	1.2355769	-1.1893947
C	-2.1564161	0.8135596	-1.4391615
C	-3.2031596	1.3325136	-0.7002037
H	-4.2258474	0.9927484	-0.8809238
C	-2.9640498	2.3068719	0.2977090
H	-3.8034245	2.7085965	0.8685058
C	-1.6808292	2.7410414	0.5561358
H	-1.4922189	3.4801941	1.3376672

1’(Bi) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1199.342362482

Bi	-1.4693692	2.6211654	0.1802858

Bi	1.3955983	2.6229885	-0.4846433
C	-0.8748033	1.1567125	1.8314537
C	-1.8966600	0.6846399	2.6360281
H	-2.9224239	1.0312661	2.4867474
C	-1.6487107	-0.2587729	3.6618778
H	-2.4742200	-0.6185594	4.2782690
C	-0.3674937	-0.7146619	3.8745911
H	-0.1607178	-1.4411035	4.6636140
C	0.7147120	-0.2499073	3.0808222
C	0.4696202	0.7125730	2.0268668
C	1.5896911	1.1560331	1.2576673
C	2.8614435	0.6826431	1.5277475
H	3.7159798	1.0287200	0.9407005
C	3.0914783	-0.2614176	2.5571610
H	4.1040120	-0.6224493	2.7449408
C	2.0358176	-0.7161617	3.3143633
H	2.1982925	-1.4428800	4.1134268
C	-1.6193746	0.9575570	-1.3801530
C	-2.8767348	0.4198995	-1.5906853
H	-3.7415047	0.8071076	-1.0458318
C	-3.0784598	-0.6431766	-2.5033733
H	-4.0800176	-1.0523697	-2.6457951
C	-2.0093852	-1.1521088	-3.2052964
H	-2.1501803	-1.9707247	-3.9145612
C	-0.7024268	-0.6244487	-3.0302221
C	-0.4861656	0.4601456	-2.0952122
C	0.8448289	0.9619731	-1.9551746
C	1.8807150	0.4292098	-2.7017882
H	2.8960191	0.8197096	-2.5955909
C	1.6610204	-0.6331764	-3.6111908
H	2.4972366	-1.0381858	-4.1835096
C	0.3935932	-1.1468922	-3.7671504
H	0.2085896	-1.9653473	-4.4663851

1a'(Bi) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2398.722703527

Bi	-2.0722851	4.1184038	-1.6374964
Bi	0.8003960	4.1270899	-2.2652032
C	-1.5009348	2.6816856	0.0393185
C	-2.5176842	2.2641032	0.8807755
H	-3.5305536	2.6574234	0.7602564
C	-2.2792741	1.3147365	1.9027099
H	-3.0987997	0.9937361	2.5479302
C	-1.0204318	0.7822447	2.0623847
H	-0.8282434	0.0293867	2.8275186
C	0.0517402	1.1889374	1.2270286
C	-0.1744942	2.1754555	0.1924853
C	0.9456465	2.5683453	-0.6034740
C	2.1919692	2.0059297	-0.3944066

H	3.0436868	2.3071832	-1.0098380
C	2.3937568	1.0181318	0.5984514
H	3.3760566	0.5613668	0.7247760
C	1.3433266	0.6259301	1.3928050
H	1.4845944	-0.1373988	2.1553556
C	-2.1777656	2.4285028	-3.1810737
C	-3.4058894	1.8078293	-3.3318819
H	-4.2711175	2.1526405	-2.7599882
C	-3.5737665	0.7078310	-4.2065798
H	-4.5492661	0.2262929	-4.2907256
C	-2.5047489	0.2514918	-4.9439147
H	-2.6199462	-0.5961147	-5.6226200
C	-1.2293284	0.8666879	-4.8373132
C	-1.0431269	1.9778339	-3.9269902
C	0.2688988	2.5345336	-3.8154734
C	1.3076786	2.0459601	-4.5889208
H	2.3090517	2.4748982	-4.5010640
C	1.1125429	0.9718149	-5.4905537
H	1.9513081	0.6006034	-6.0815574
C	-0.1304086	0.3908541	-5.6012253
H	-0.2915303	-0.4507958	-6.2780223
Bi	2.0722871	-4.1184026	1.6375087
Bi	-0.8003967	-4.1270888	2.2651992
C	1.5009451	-2.6816877	-0.0393123
C	2.5176983	-2.2641080	-0.8807664
H	3.5305658	-2.6574328	-0.7602457
C	2.2792926	-1.3147451	-1.9027051
H	3.0988150	-0.9937676	-2.5479411
C	1.0204526	-0.7822483	-2.0623830
H	0.8282692	-0.0293895	-2.8275179
C	-0.0517239	-1.1889411	-1.2270327
C	0.1745055	-2.1754573	-0.1924867
C	-0.9456384	-2.5683446	0.6034692
C	-2.1919596	-2.0059279	0.3943961
H	-3.0436888	-2.3072090	1.0097978
C	-2.3937413	-1.0181272	-0.5984600
H	-3.3760349	-0.5613466	-0.7247755
C	-1.3433089	-0.6259323	-1.3928140
H	-1.4845720	0.1373965	-2.1553657
C	2.1777588	-2.4285000	3.1810851
C	3.4058816	-1.8078263	3.3318990
H	4.2711127	-2.1526373	2.7600096
C	3.5737552	-0.7078312	4.2066020
H	4.5492599	-0.2263071	4.2907696
C	2.5047321	-0.2514872	4.9439259
H	2.6199209	0.5961323	5.6226163
C	1.2293126	-0.8666852	4.8373195
C	1.0431165	-1.9778312	3.9269956
C	-0.2689085	-2.5345315	3.8154716
C	-1.3076923	-2.0459594	4.5889141

H	-2.3090648	-2.4748969	4.5010513
C	-1.1125611	-0.9718144	5.4905483
H	-1.9513287	-0.6006057	6.0815505
C	0.1303871	-0.3908474	5.6012206
H	0.2914934	0.4508333	6.2779831

1b'(Bi) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2398.714843365

Bi	-2.4509643	-0.3671577	-1.9500435
Bi	0.4076844	-0.3617618	-2.6200174
C	-1.8443284	-1.7654214	-0.2443097
C	-2.8554560	-2.2007739	0.5952130
H	-3.8796098	-1.8469413	0.4524099
C	-2.5995580	-3.1124634	1.6472321
H	-3.4168579	-3.4392875	2.2921989
C	-1.3208606	-3.5808031	1.8499506
H	-1.1085111	-4.2843546	2.6578339
C	-0.2484543	-3.1559310	1.0210080
C	-0.5009790	-2.2190364	-0.0549333
C	0.6107768	-1.7975385	-0.8497985
C	1.8813391	-2.2800324	-0.5867409
H	2.7307216	-1.9508684	-1.1907621
C	2.1179868	-3.2067566	0.4581508
H	3.1301038	-3.5725074	0.6384582
C	1.0714439	-3.6309064	1.2451135
H	1.2404044	-4.3379942	2.0600926
C	-2.5852944	-2.1161903	-3.4247476
C	-3.8336376	-2.6883448	-3.5979694
H	-4.7001730	-2.2943677	-3.0603182
C	-4.0246859	-3.7938404	-4.4612568
H	-5.0194678	-4.2284247	-4.5739368
C	-2.9540143	-4.3115052	-5.1546580
H	-3.0868467	-5.1621710	-5.8269477
C	-1.6559887	-3.7514116	-5.0179329
C	-1.4511592	-2.6244675	-4.1319046
C	-0.1288102	-2.0906585	-4.0250930
C	0.9086644	-2.6356515	-4.7615576
H	1.9176897	-2.2223659	-4.6821791
C	0.7007205	-3.7382525	-5.6248157
H	1.5386578	-4.1504027	-6.1897538
C	-0.5577785	-4.2828785	-5.7452965
H	-0.7336584	-5.1333992	-6.4078230
Bi	2.4509648	0.3671566	1.9500444
Bi	-0.4076838	0.3617604	2.6200188
C	1.8443289	1.7654202	0.2443107
C	2.8554563	2.2007727	-0.5952121
H	3.8796101	1.8469401	-0.4524092
C	2.5995582	3.1124621	-1.6472313

H	3.4168579	3.4392858	-2.2921985
C	1.3208608	3.5808019	-1.8499494
H	1.1085117	4.2843555	-2.6578310
C	0.2484545	3.1559296	-1.0210069
C	0.5009794	2.2190351	0.0549345
C	-0.6107761	1.7975372	0.8497999
C	-1.8813385	2.2800309	0.5867423
H	-2.7307210	1.9508668	1.1907636
C	-2.1179864	3.2067548	-0.4581494
H	-3.1301036	3.5725051	-0.6384572
C	-1.0714437	3.6309051	-1.2451121
H	-1.2404030	4.3379990	-2.0600861
C	2.5852946	2.1161887	3.4247490
C	3.8336370	2.6883462	3.5979671
H	4.7001524	2.2944364	3.0602345
C	4.0246876	3.7938342	4.4612637
H	5.0194740	4.2284034	4.5739619
C	2.9540158	4.3114997	5.1546642
H	3.0868564	5.1621385	5.8269864
C	1.6559880	3.7514138	5.0179300
C	1.4511591	2.6244672	4.1319046
C	0.1288104	2.0906574	4.0250941
C	-0.9086648	2.6356522	4.7615565
H	-1.9177020	2.2224042	4.6821331
C	-0.7007198	3.7382496	5.6248188
H	-1.5386535	4.1503885	6.1897705
C	0.5577785	4.2828784	5.7452963
H	0.7336608	5.1333911	6.4078323

1c'(Bi) optimized at the BP+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2398.713352310

Bi	-0.5660908	0.8920578	3.5041966
Bi	2.2782735	0.9657548	2.7720000
C	0.0981166	-0.6022644	5.1089836
C	-0.8943124	-1.1156345	5.9256986
H	-1.9304513	-0.7876018	5.8076376
C	-0.6038750	-2.0772682	6.9231876
H	-1.4074287	-2.4685958	7.5495021
C	0.6909428	-2.5112042	7.0964921
H	0.9305489	-3.2512031	7.8634415
C	1.7446876	-2.0055339	6.2894741
C	1.4553353	-1.0242023	5.2646303
C	2.5466296	-0.5382548	4.4790763
C	3.8337161	-0.9920526	4.7090514
H	4.6668632	-0.6151695	4.1099387
C	4.1079158	-1.9542871	5.7105419
H	5.1319331	-2.2980807	5.8664365
C	3.0803206	-2.4489092	6.4814397

H	3.2769690	-3.1902041	7.2592728
C	-0.7165730	-0.7537264	1.9287426
C	-1.9657368	-1.3160978	1.7417338
H	-2.8300150	-0.9341025	2.2902113
C	-2.1601160	-2.3947785	0.8471740
H	-3.1544264	-2.8279940	0.7264874
C	-1.0916239	-2.8917265	0.1340057
H	-1.2243132	-3.7298464	-0.5540162
C	0.2042999	-2.3271978	0.2738879
C	0.4123696	-1.2288064	1.1932989
C	1.7312146	-0.6910283	1.2993620
C	2.7609250	-1.1936729	0.5247880
H	3.7636020	-0.7652717	0.5957972
C	2.5511960	-2.2696628	-0.3688170
H	3.3829168	-2.6539161	-0.9616338
C	1.2967183	-2.8273249	-0.4835294
H	1.1213320	-3.6652884	-1.1621272
Bi	0.5660906	-0.8920575	-3.5041961
Bi	-2.2782737	-0.9657541	-2.7719996
C	-0.0981163	0.6022655	-5.1089826
C	0.8943127	1.1156354	-5.9256976
H	1.9304475	0.7875837	-5.8076534
C	0.6038762	2.0772729	-6.9231831
H	1.4074335	2.4686168	-7.5494830
C	-0.6909429	2.5112025	-7.0964936
H	-0.9305505	3.2511943	-7.8634493
C	-1.7446875	2.0055336	-6.2894745
C	-1.4553351	1.0242035	-5.2646292
C	-2.5466296	0.5382555	-4.4790759
C	-3.8337160	0.9920535	-4.7090510
H	-4.6668624	0.6151744	-4.1099347
C	-4.1079156	1.9542884	-5.7105411
H	-5.1319306	2.2980931	-5.8664258
C	-3.0803215	2.4489039	-6.4814448
H	-3.2769735	3.1901807	-7.2592944
C	0.7165729	0.7537267	-1.9287421
C	1.9657368	1.3160981	-1.7417333
H	2.8300149	0.9341027	-2.2902108
C	2.1601160	2.3947788	-0.8471736
H	3.1544264	2.8279945	-0.7264872
C	1.0916240	2.8917269	-0.1340053
H	1.2243133	3.7298470	0.5540162
C	-0.2042998	2.3271982	-0.2738874
C	-0.4123696	1.2288067	-1.1932983
C	-1.7312146	0.6910287	-1.2993613
C	-2.7609250	1.1936734	-0.5247873
H	-3.7636021	0.7652724	-0.5957967
C	-2.5511959	2.2696633	0.3688177
H	-3.3829166	2.6539166	0.9616346
C	-1.2967181	2.8273254	0.4835300

H -1.1213319 3.6652891 1.1621277

1'(Bi) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -1198.027409464

Bi	-1.4690301	2.5913643	0.1817966
Bi	1.3965983	2.5929452	-0.4829679
C	-0.8719186	1.1403242	1.8411216
C	-1.8920948	0.6764992	2.6527324
H	-2.9190034	1.0191905	2.4978045
C	-1.6413903	-0.2509665	3.6914899
H	-2.4660292	-0.6049032	4.3133559
C	-0.3588028	-0.6990798	3.9105796
H	-0.1481337	-1.4136456	4.7101036
C	0.7212999	-0.2420063	3.1105918
C	0.4733341	0.7037055	2.0433068
C	1.5914718	1.1397699	1.2681769
C	2.8647708	0.6749038	1.5460827
H	3.7180870	1.0171109	0.9538654
C	3.0976502	-0.2530678	2.5885331
H	4.1117994	-0.6079907	2.7822472
C	2.0432375	-0.7002758	3.3514407
H	2.2065527	-1.4150889	4.1617403
C	-1.6203916	0.9400087	-1.3885829
C	-2.8795814	0.4098554	-1.6075803
H	-3.7429208	0.7939215	-1.0570156
C	-3.0848042	-0.6388790	-2.5349806
H	-4.0881738	-1.0427518	-2.6837786
C	-2.0173351	-1.1409746	-3.2436926
H	-2.1594543	-1.9490466	-3.9655176
C	-0.7092853	-0.6203791	-3.0607017
C	-0.4894407	0.4491142	-2.1104873
C	0.8426485	0.9441493	-1.9629677
C	1.8764584	0.4186972	-2.7177522
H	2.8930644	0.8058679	-2.6056129
C	1.6533178	-0.6292844	-3.6419305
H	2.4883764	-1.0291573	-4.2205367
C	0.3842486	-1.1359571	-3.8049494
H	0.1948743	-1.9439733	-4.5159145

1a'(Bi) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2396.081988177

Bi	-2.0517665	4.1409537	-1.6753944
Bi	0.8030705	4.2149224	-2.3774145
C	-1.3988388	2.7077185	-0.0268067
C	-2.3964550	2.2167139	0.7967144

H	-3.4329768	2.5376062	0.6586389
C	-2.1087362	1.2831672	1.8198398
H	-2.9147845	0.8959599	2.4463695
C	-0.8151593	0.8572359	2.0125219
H	-0.5810772	0.1291356	2.7908551
C	0.2411351	1.3462826	1.2008111
C	-0.0419752	2.2982658	0.1485301
C	1.0556013	2.7600279	-0.6399760
C	2.3412261	2.3138632	-0.3901086
H	3.1773673	2.6741984	-0.9962665
C	2.6051298	1.3759865	0.6354170
H	3.6247772	1.0228783	0.8018597
C	1.5727899	0.9036751	1.4118164
H	1.7614779	0.1735882	2.2003579
C	-2.1796456	2.4768547	-3.2399655
C	-3.4222937	1.8963328	-3.4255209
H	-4.2872726	2.2557332	-2.8611207
C	-3.6072651	0.8232053	-4.3295332
H	-4.5967055	0.3769600	-4.4469214
C	-2.5366211	0.3466061	-5.0513216
H	-2.6618540	-0.4839264	-5.7500284
C	-1.2454490	0.9189022	-4.9048028
C	-1.0464284	2.0128427	-3.9773730
C	0.2723575	2.5498959	-3.8525818
C	1.3116920	2.0400219	-4.6110988
H	2.3186900	2.4553644	-4.5144056
C	1.1094010	0.9686001	-5.5135409
H	1.9502045	0.5794615	-6.0910616
C	-0.1456074	0.4207559	-5.6520847
H	-0.3172767	-0.4104625	-6.3400473
Bi	2.0518349	-4.1409196	1.6754378
Bi	-0.8030302	-4.2149525	2.3773410
C	1.3989366	-2.7077036	0.0268214
C	2.3965700	-2.2167038	-0.7966822
H	3.4330688	-2.5376988	-0.6586712
C	2.1088739	-1.2831571	-1.8198140
H	2.9149281	-0.8959965	-2.4463656
C	0.8153016	-0.8572228	-2.0125222
H	0.5812366	-0.1291208	-2.7908600
C	-0.2410113	-1.3462759	-1.2008386
C	0.0420749	-2.2982620	-0.1485542
C	-1.0555218	-2.7600373	0.6399149
C	-2.3411397	-2.3138669	0.3900245
H	-3.1772801	-2.6741291	0.9962262
C	-2.6050187	-1.3759809	-0.6354984
H	-3.6246495	-1.0228117	-0.8019123
C	-1.5726618	-0.9036722	-1.4118766
H	-1.7613288	-0.1735846	-2.2004219
C	2.1796078	-2.4768294	3.2400283
C	3.4222383	-1.8962885	3.4256471

H	4.2872505	-2.2556719	2.8612865
C	3.6071504	-0.8231689	4.3296806
H	4.5965849	-0.3769294	4.4471430
C	2.5364655	-0.3465965	5.0514255
H	2.6616685	0.4838798	5.7502046
C	1.2453063	-0.9189031	4.9048313
C	1.0463482	-2.0128420	3.9773876
C	-0.2724215	-2.5499192	3.8525353
C	-1.3118011	-2.0400666	4.6110034
H	-2.3187869	-2.4554261	4.5142609
C	-1.1095756	-0.9686296	5.5134420
H	-1.9504138	-0.5795053	6.0909217
C	0.1454190	-0.4207717	5.6520562
H	0.3170446	0.4104376	6.3400407

1b'(Bi) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2396.074567262

Bi	-2.4578194	-0.4212945	-1.9977747
Bi	0.4022353	-0.4228267	-2.6735421
C	-1.8451152	-1.7951562	-0.2755920
C	-2.8546040	-2.2192548	0.5711888
H	-3.8804952	-1.8716433	0.4205506
C	-2.5958101	-3.1116672	1.6383653
H	-3.4126600	-3.4318786	2.2881747
C	-1.3153097	-3.5703704	1.8494612
H	-1.0990654	-4.2602317	2.6688646
C	-0.2446248	-3.1543702	1.0146111
C	-0.5006024	-2.2387935	-0.0776033
C	0.6089144	-1.8294787	-0.8808625
C	1.8817685	-2.2993455	-0.6070116
H	2.7297280	-1.9769881	-1.2179348
C	2.1221842	-3.2046476	0.4548033
H	3.1361427	-3.5636719	0.6420893
C	1.0765432	-3.6201991	1.2473775
H	1.2463414	-4.3132938	2.0749264
C	-2.5972413	-2.1663631	-3.4721972
C	-3.8485975	-2.7303159	-3.6489812
H	-4.7124597	-2.3346752	-3.1071146
C	-4.0461391	-3.8276482	-4.5203446
H	-5.0436870	-4.2564624	-4.6355750
C	-2.9787582	-4.3447883	-5.2185841
H	-3.1150804	-5.1896964	-5.8982420
C	-1.6784316	-3.7922494	-5.0786758
C	-1.4670250	-2.6742644	-4.1843633
C	-0.1425595	-2.1482669	-4.0750487
C	0.8909937	-2.6918991	-4.8176583
H	1.9021090	-2.2826986	-4.7360677
C	0.6766781	-3.7861946	-5.6890616

H	1.5121338	-4.1979998	-6.2588869
C	-0.5844976	-4.3232993	-5.8117070
H	-0.7671588	-5.1678744	-6.4808333
Bi	2.4578241	0.4212991	1.9977727
Bi	-0.4022325	0.4228248	2.6735330
C	1.8451213	1.7951579	0.2755878
C	2.8546099	2.2192524	-0.5711953
H	3.8805016	1.8716435	-0.4205544
C	2.5958165	3.1116621	-1.6383743
H	3.4126741	3.4319041	-2.2881589
C	1.3153156	3.5703629	-1.8494735
H	1.0990717	4.2602177	-2.6688824
C	0.2446313	3.1543675	-1.0146203
C	0.5006087	2.2387946	0.0775975
C	-0.6089084	1.8294830	0.8808579
C	-1.8817618	2.2993529	0.6070080
H	-2.7297214	1.9769990	1.2179328
C	-2.1221766	3.2046529	-0.4548087
H	-3.1361348	3.5636773	-0.6420961
C	-1.0765355	3.6202004	-1.2473850
H	-1.2463248	4.3133328	-2.0749042
C	2.5972383	2.1663659	3.4721982
C	3.8485915	2.7303257	3.6489804
H	4.7124337	2.3347647	3.1070237
C	4.0461314	3.8276482	4.5203566
H	5.0436792	4.2564605	4.6355944
C	2.9787504	4.3447760	5.2186050
H	3.1150830	5.1896365	5.8983199
C	1.6784219	3.7922455	5.0786798
C	1.4670194	2.6742631	4.1843633
C	0.1425559	2.1482606	4.0750474
C	-0.8909997	2.6918878	4.8176572
H	-1.9021199	2.2827044	4.7360412
C	-0.6766880	3.7861808	5.6890646
H	-1.5121494	4.1979947	6.2588753
C	0.5844883	4.3232814	5.8117218
H	0.7671550	5.1678269	6.4808840

1c'(Bi) optimized at the PBE+D3/def2-TZVP level of theory:
Energy (in Hartree) and atomic coordinates (in Å):

Energy = -2396.073958334

Bi	-0.5699116	0.7725418	3.5532081
Bi	2.2740331	0.8569786	2.8143947
C	0.1111715	-0.6757695	5.1882680
C	-0.8739103	-1.1736640	6.0229741
H	-1.9138024	-0.8590118	5.8965820
C	-0.5714868	-2.1006465	7.0485071
H	-1.3698611	-2.4812434	7.6887895
C	0.7281200	-2.5148203	7.2317930

H	0.9787797	-3.2284556	8.0206246
C	1.7742184	-2.0228174	6.4075450
C	1.4725667	-1.0773366	5.3541707
C	2.5566052	-0.6038848	4.5524469
C	3.8489440	-1.0355725	4.7943006
H	4.6767174	-0.6661112	4.1822244
C	4.1352682	-1.9635864	5.8234912
H	5.1637338	-2.2912588	5.9881241
C	3.1143139	-2.4454708	6.6106179
H	3.3189357	-3.1606962	7.4112008
C	-0.7142975	-0.8813351	1.9861763
C	-1.9645491	-1.4398436	1.7927753
H	-2.8259992	-1.0697479	2.3552241
C	-2.1643505	-2.4950800	0.8721767
H	-3.1605948	-2.9234366	0.7445386
C	-1.0997140	-2.9747240	0.1422809
H	-1.2367296	-3.7918002	-0.5706865
C	0.1984088	-2.4196062	0.2948923
C	0.4116142	-1.3434992	1.2386845
C	1.7314855	-0.8101056	1.3522806
C	2.7595408	-1.3032330	0.5693899
H	3.7644590	-0.8798695	0.6496269
C	2.5449430	-2.3591603	-0.3468153
H	3.3760320	-2.7350262	-0.9470367
C	1.2876332	-2.9060165	-0.4754615
H	1.1059872	-3.7249123	-1.1762768
Bi	0.5699093	-0.7725434	-3.5532065
Bi	-2.2740360	-0.8569777	-2.8143949
C	-0.1111717	0.6757660	-5.1882688
C	0.8739110	1.1736583	-6.0229751
H	1.9138113	0.8590478	-5.8965463
C	0.5714881	2.1006353	-7.0485132
H	1.3698626	2.4812281	-7.6887979
C	-0.7281183	2.5148095	-7.2318009
H	-0.9787807	3.2284249	-8.0206496
C	-1.7742160	2.0228166	-6.4075461
C	-1.4725657	1.0773378	-5.3541696
C	-2.5566050	0.6038883	-4.5524455
C	-3.8489428	1.0355795	-4.7942984
H	-4.6767203	0.6661007	-4.1822383
C	-4.1352642	1.9635995	-5.8234842
H	-5.1637225	2.2913107	-5.9880858
C	-3.1143116	2.4454681	-6.6106228
H	-3.3189354	3.1606758	-7.4112210
C	0.7142952	0.8813353	-1.9861766
C	1.9645467	1.4398446	-1.7927768
H	2.8259965	1.0697493	-2.3552264
C	2.1643483	2.4950813	-0.8721787
H	3.1605925	2.9234384	-0.7445416
C	1.0997122	2.9747245	-0.1422818

H	1.2367282	3.7918007	0.5706857
C	-0.1984104	2.4196060	-0.2948920
C	-0.4116161	1.3434991	-1.2386842
C	-1.7314874	0.8101052	-1.3522797
C	-2.7595423	1.3032322	-0.5693882
H	-3.7644605	0.8798685	-0.6496248
C	-2.5449441	2.3591591	0.3468173
H	-3.3760327	2.7350246	0.9470395
C	-1.2876344	2.9060156	0.4754628
H	-1.1059882	3.7249112	1.1762782

Table S2. Fragment-fragment interaction energies [kJ/mol] for the crystal structure motifs (Sb).

		ds···np	ds···np'	ds···ds	np···np	np···np'
1a(Sb)	$E^{(1)}_{el}$	-0.93	0.08	0.04	-11.18	-9.03
	$E^{(1)}_{exch}$	2.79	0.00	0.00	40.77	18.29
	$E^{(2)}_{ind}$	-0.95	-0.01	-0.002	-16.73	-5.22
	$E^{(2)}_{ind\text{-}exch}$	0.72	0.00	0.00	15.69	4.35
	$E^{(2)}_{disp}$	-8.61	-0.39	-0.34	-53.77	-26.32
	$E^{(2)}_{disp\text{-}exch}$	0.53	0.00	0.00	7.70	2.77
	δ(HF)	-0.11	0.00	0.00	-1.15	-1.55
	E_{int}(DFT-SAPT)	-6.56	-0.32	-0.30	-18.66	-16.71
	E_{int}(BP+D3)	-6.15	-0.32	-0.22	-33.21	-24.72
	E_{int}(PBE+D3)	-8.50	-0.30	-0.22	-24.36	-22.01
	E_{int}(SCS-MP2)	-6.56	-0.377	-0.32	-26.62	-18.09
1b(Sb)	$E^{(1)}_{el}$	-26.05	0.15	-2.82	-3.53	-0.87
	$E^{(1)}_{exch}$	49.89	0.01	8.31	5.94	0.05
	$E^{(2)}_{ind}$	-48.31	-0.02	-6.68	-2.23	-0.09
	$E^{(2)}_{ind\text{-}exch}$	39.41	0.002	4.70	1.85	0.01
	$E^{(2)}_{disp}$	-49.38	-1.12	-16.71	-14.15	-2.34
	$E^{(2)}_{disp\text{-}exch}$	8.84	0.003	1.45	1.19	0.02
	δ(HF)	6.43	0.001	1.11	-0.49	-0.01
	E_{int}(DFT-SAPT)	-19.17	-0.97	-10.64	-11.41	-3.23
	E_{int}(BP+D3)	-23.54	-0.83	-14.76	-12.74	-3.01
	E_{int}(PBE+D3)	-15.97	-1.13	-12.10	-14.79	-3.82
	E_{int}(SCS-MP2)	-20.51	-1.02	-10.41	-12.26	-3.38
1c(Sb)	$E^{(1)}_{el}$	-21.37	-0.08	-0.15	-8.61	-0.49
	$E^{(1)}_{exch}$	39.35	0.00	0.12	33.76	0.05
	$E^{(2)}_{ind}$	-41.40	-0.003	-0.05	-14.25	-0.06
	$E^{(2)}_{ind\text{-}exch}$	32.35	0.00	0.02	13.25	0.01
	$E^{(2)}_{disp}$	-40.61	-0.35	-2.32	-48.13	-1.97
	$E^{(2)}_{disp\text{-}exch}$	6.38	0.00	0.03	6.58	0.01
	δ(HF)	8.06	0.00	0.00	-2.51	-0.01
	E_{int}(DFT-SAPT)	-17.24	-0.43	-2.34	-19.92	-2.46
	E_{int}(BP+D3)	-23.76	-0.43	-1.56	-30.06	-2.30
	E_{int}(PBE+D3)	-18.02	-0.41	-2.61	-23.70	-2.98
	E_{int}(SCS-MP2)	-19.13	-0.47	-2.43	-25.12	-2.57

Table S3. Structural parameters (bond lengths [Å] and angles [°]) of the geometry-optimized dimers.

E			E- E	C- E-C	E… E	E…π	π…π	CH…π
P	BP-d3	1a'	2.264	99	8.433	5.610/5.613	3.617	2.445/2.452
		1b'	2.261	98.9/99.1	4.627/4.633	3.459/3.459/3.499/3.503	4.896/4.906	---
		1c'	2.261	99.5/99.7	6.574	4.203/4.249	3.703	---
	PBE-d3	1a'	2.257	100.1	8.537	5.753/5.790	3.866	2.566/2.628
		1c'	2.255	100.4/100.5	6.686	4.378/4.435	3.914	---
As	BP-d3	1a'	2.47	95.8/96.1	8.715	5.709/5.793	3.63	2.397/2.520
		1b'	2.47	95.0/95.5	4.78	3.500/3.613	5.045	---
		1c'	2.467	96.0/96.1	6.665	4.200/4.207	3.727	---
	PBE-d3	1a'	2.465	96.8	8.845	5.920/5.930	3.866	2.574/2.591
		1c'	2.463	96.9	6.731	4.347/4,353	3.937	---
Sb	BP-d3	1a'	2.808	93.2/93.6	9.068	5.872/5.943	3.636	2.407/2.507
		1b'	2.806	92.4/92.9	5.128/5.133	3.735/3.901	5.345/5.350	---
		1c'	2.805	93.3/93.4	6.922/6.924	4.256/4.257/4.302/4.303	3.792/3.793	---
	PBE-d3	1a'	2.807	94.4	9.211	6.091/6.094	3.881	2.584/2.588
		1b'	2.807	93.5/93.8	5.317	3.882/3.883/4.029/4.030	5.364/5.366	---
		1c'	2.805	94.3/94.4	6.961/6.964	4.392/4.394/4.437/4.438	4.025/4.026	---
Bi	BP-d3	1a'	2.941	91.9/92.4	9.211	5.924/6.002	3.637	2.412/2.527
		1b'	2.936	91.2/91.7	5.059	3.720/3.898	5.531	---
		1c'	2.938	91.9	6.766	4.111/4.128	3.897	---
	PBE-d3	1a'	2.941	93.0/93.1	9.370	6.156/6.164	3.880	2.582/2.597
		1b'	2.939	92.2/92.5	5.173	3.813/3.978	5.543	---
		1c'	2.940	92.8/92.9	6.790	4.238/4.246	4.111	---

Table S4. Fragment-fragment interaction energies [kJ/mol] for the BP+D3-optimized structural motifs **1b'**(E) (E = P, As, Sb, Bi).

	P		As		Sb		Bi	
	de···np	de···de	de···np	de···de	de···np	de···de	de···np	de···de
$E^{(1)}_{el}$	-12.84	-0.89	-17.92	-0.41	-18.84	-1.24	-21.38	-3.80
$E^{(1)}_{exch}$	38.97	2.23	44.83	2.44	35.35	2.59	36.30	3.92
$E^{(2)}_{ind}$	-19.23	-0.68	-29.31	-1.02	-29.63	-1.74	-34.76	-4.01
$E^{(2)}_{ind\text{-}exch}$	17.72	0.43	27.53	0.83	24.13	1.16	27.42	2.62
$E^{(2)}_{disp}$	-41.16	-7.10	-44.87	-8.15	-42.75	-9.45	-44.68	-12.23
$E^{(2)}_{disp\text{-}exch}$	6.73	0.36	7.40	0.43	6.66	0.52	6.93	0.83
δ(HF)	-2.85	-0.20	-3.49	-0.23	3.02	0.23	5.21	0.72
E_{int}(DFT-SAPT)	-12.68	-5.83	-15.83	-6.11	-22.05	-7.93	-24.95	-11.95
E_{int}(BP+D3)	-18.95	-6.56	-25.26	-8.75	-23.40	-11.05	-27.97	-18.31
E_{int}(PBE+D3)	-11.85	-7.77	-15.31	-8.39	-17.06	-9.62	-19.77	-14.12
E_{int}(SCS-MP2)	-14.07	-5.25	-17.12	-5.92	-23.98	-8.13	-28.19	-12.79

Figure S6. de···de and de···np interaction energies for the BP+D3-optimized structural motifs **1b'**(E) (E = P, As, Sb, Bi).