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SUPPORTING INFORMATION

The Mechanism of the Insertion Reactions of Silylenes

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Table S1. Reaction Energies, Reaction Gibbs Free Energies, Reaction Activation Energies and Reaction Activation Gibbs Free Energies of the $SiH_2+H_2=SiH_4$ (**A1**) Insertion Reaction in various Levels of computation in kJ/mol

Method/Level	**Geometry**	ΔE	ΔG	$\Delta E^{\ddagger}$	$\Delta G^{\ddagger}$
B3LYP/cc-pVTZ	B3LYP/cc-pVTZ	-246.8	-196.7	-5.0	33.5
MP2/cc-pVTZ	MP2/cc-pVTZ	-261.3	-210.4	-4.3	34.3
CCSD/cc-pVTZ	B3LYP/cc-pVTZ	-247.3	-196.2	11.2	50.1
CCSD(T)/cc-pVTZ	B3LYP/cc-pVTZ	-247.3	-194.4	11.2	50.2
CCSD/cc-pVQZ	B3LYP/cc-pVTZ	-247.6	-196.7	2.0	40.5
CCSD(T)/cc-pVQZ	B3LYP/cc-pVTZ	-254.2	-	5.5	-
CCSD/cc-pVTZ	CCSD/cc-pVTZ	-254.5	-	-4.6	-
CCSD(T)/6-31g(d,p)	CCSD(T)/6-31g(d,p)		-	25.0*	-

* Wang and Ma computational results (reference 4b)

Table S2. Reaction Energies, Reaction Gibbs Free Energies of **A1**, **B1**, **G1** Insertion Reaction in various Levels computed by Wang and Ma (ref. 4b) in kJ/mol

Method/Level	**Geometry**	**A1**	**B1**	**G1**	**A1**	**B1**	**G1**
		$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}$	ΔE	ΔE	ΔE
B3LYP/6-311g**	B3LYP/6-311g**	20.2	190.7	265.5	-212.2	-97.7	-27.8
MP2/6-31g**	MP2/6-31g**	25.6	222.1	313.9	-236.6	-105.4	-16.3
CASSCF(6,6)/6-31g**	CASSCF(6,6)/6-31g**	70.6	263.3	342.3	-221.7	-62.0	40.2
CASPT2(6,6)/6-31g**	CASPT2(6,6)/6-31g**	22.7	212.4	318.2	-251.9	-124.7	-29.4
B3LYP/cc- pVTZ [#]	B3LYP/cc-pVTZ	-5.0	177.7	259.5	-246.8	-119.9	-43.7
MP2/cc- pVTZ [#]	MP2/cc-pVTZ	-4.3	181.3	-	-261.3	-137.1	-50.4
CCSD/cc- pVTZ [#]	B3LYP/cc-pVTZ	11.2	185.3	-	-247.3	-133.8	-

[#] Our computational results

Figure S1. Correlation of Insertion Reaction Energies and Activation Energies Calculated at the B3LYP/cc-pVTZ Level with the Energies Calculated at MP2/cc-pVTZ and CCSD/cc-pVTZ//B3LYP/cc-pVTZ Levels

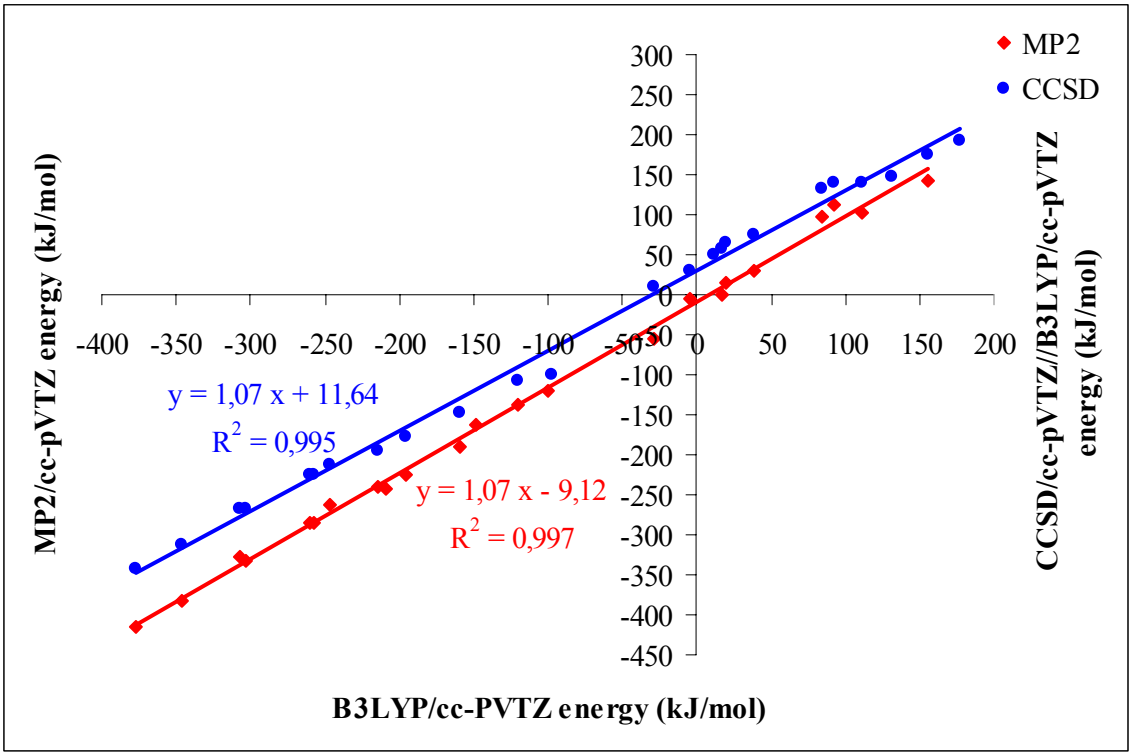


Figure S2. The reaction of SiH_2 (**A**) with H_2 (**1**) (enegries Calculated at the B3LYP/cc-pVTZ Level)

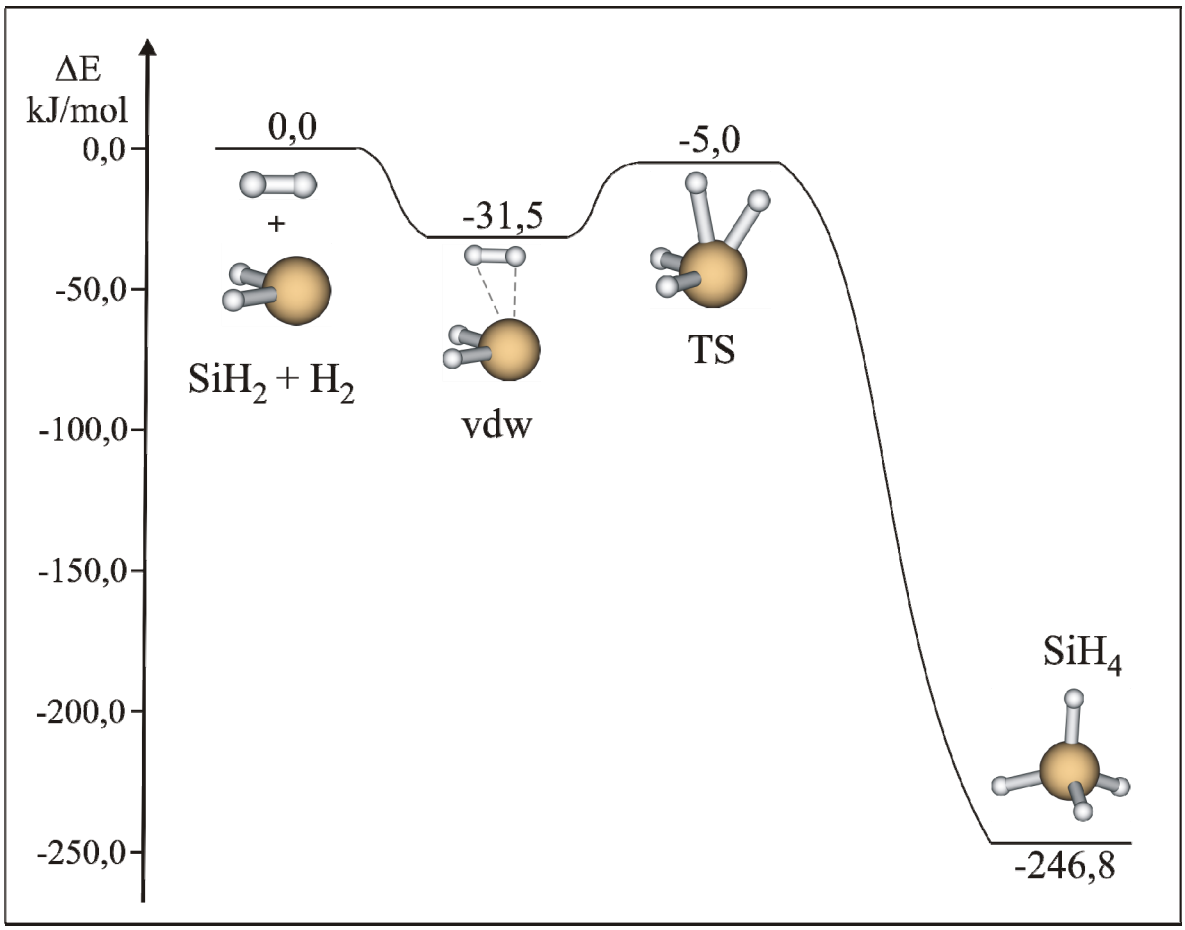
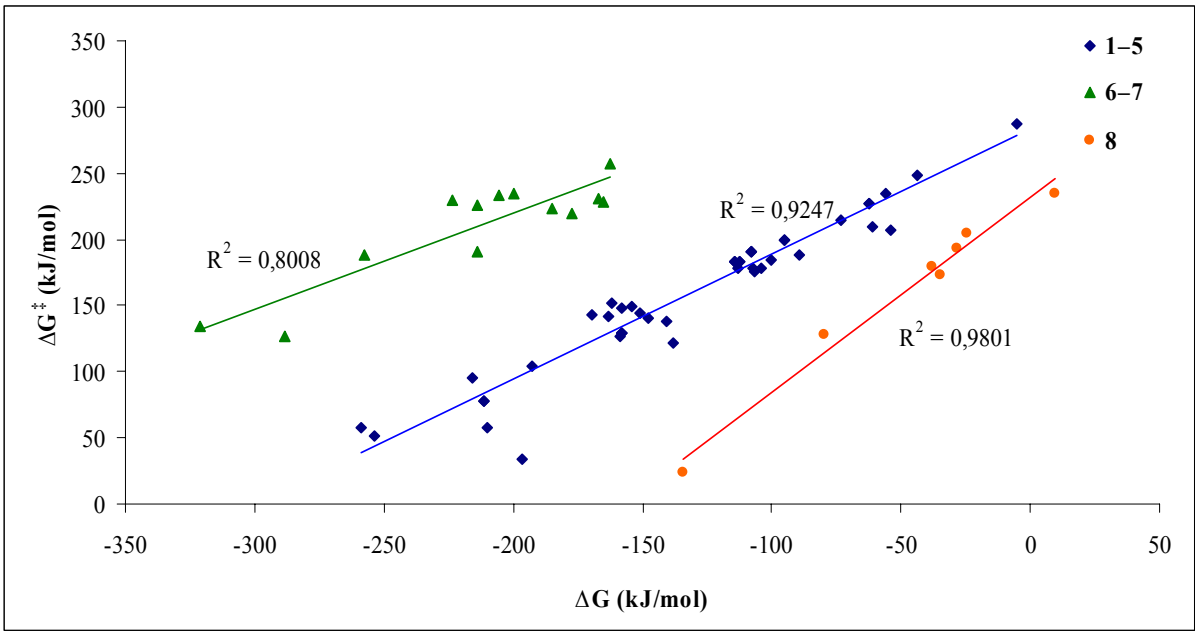
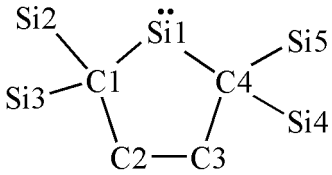
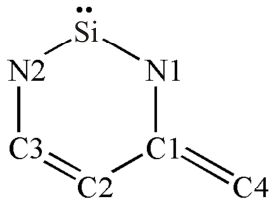
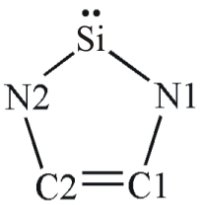


Figure S3. Correlation between the Reaction Gibbs Free Energies and Activation Gibbs Free Energies

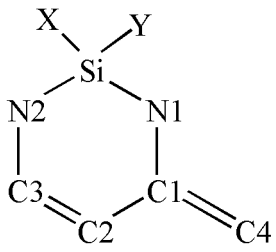
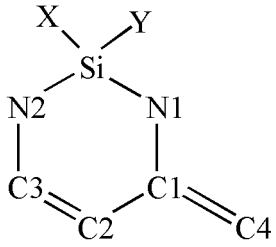
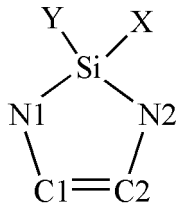


Calculated at the B3LYP/cc-pVTZ Level

Table S3-S5. Computed and Crystallographic Geometrial data (bondlength in pm, angles in deg.)

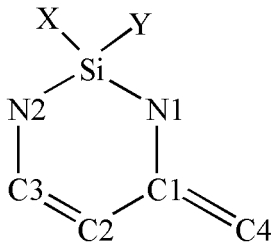
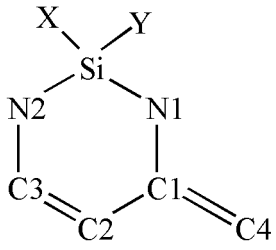
		Crystallographic data°	Computed geometry at B3LYP/cc-pVTZ Level
 **C**	Si1-C1	1,911	1,925
	Si1-C4	1,904	1,925
	C1-Si2	1,901	1,891
	C1-Si3	1,911	1,911
	C4-Si4	1,901	1,891
	C4-Si5	1,911	1,911
	C1-C2	1,569	1,558
	C2-C3	1,530	1,532
	C3-C4	1,568	1,558
	C-Si-C	93,88°	91,39°
 **D**	Si-N1	171.9	173.7
	Si-N2	171.9	173.7
	N1-C1	148.9	146.7
	N2-C2	148.9	146.7
	C1-C2	-	153.7
	N-Si-N	92.0°	88.8°
 **F**	Si-N1	1.7344	1.7387
	Si-N2	1.7353	1.7533
	N1-C1	1.4155	1.4115
	C1-C2	1.4019	1.4544
	C1-C4	1.4125	1.3457
	C2-C3	1.3896	1.3428
	N2-C3	1.4171	1.3896
	N-Si-N	99.31°	96.24°
 **G**	Si-N1	175.3	176.8
	Si-N2	175.3	176.8
	N1-C1	140.0	138.6
	N2-C2	140.0	138.6
	C1-C2	134.7	135.1
	N-Si-N	90.5°	85.2°

Calculated at the B3LYP/cc-pVTZ level

		Crystallographic data°	Computed geometry at B3LYP/cc-pVTZ Level
 **Pr-F2*** X=O, Y=H	Si-N1	178,0	172,7
	Si-N2	180,1	173,9
	N1-C1	139,3	141,5
	C1-C2	142,2	146,0
	C1-C4	140,4	135,1
	C2-C3	137,9	134,9
	N2-C3	137,9	139,5
	Si-X	163,2	166,0
	N-Si-N	96,4	101,1
 **Pr-F4** X=N, Y=H	Si-N1	172.4	172,7
	Si-N2	172.6	174,1
	N1-C1	141.1	140,6
	C1-C2	139.9	145,6
	C1-C4	141.3	134,7
	C2-C3	141.0	134,4
	N2-C3	140.6	138,8
	Si-X	165.3	170,8
	Si-Y	144.7	148,5
	N-Si-N	103.1	100,1
 **Pr-G2** X=O, Y=H	Si-N1	173,9	173,6
	Si-N2	173,5	173,6
	N1-C1	142,7	141,1
	N2-C2	142,8	141,1
	C1-C2	134,7	134,0
	Si-X	162,7	165,6
	N-Si-N	93,5	90,3

Calculated at the B3LYP/cc-pVTZ level

* Crystallographic data of the dimer of Pr-F2

		Crystallographic data°	Computed geometry at B3LYP/cc-pVTZ Level
 **Pr-F5** X=N, Y=H	Si-N1	172.5	172,6
	Si-N2	173.0	173,6
	N1-C1	141.3	140,6
	C1-C2	140.2	145,5
	C1-C4	141.7	134,7
	C2-C3	140.1	134,4
	N2-C3	141.5	138,7
	Si-X	167.9	171,7
	Si-Y	139.2	148,6
	N-Si-N	102.8	100,6
 **Pr-F8** X=Y=P	Si-N1	172,4	172,5
	Si-N2	172,8	173,6
	N1-C1	142,2	141,0
	C1-C2	141,2	145,5
	C1-C4	141,6	134,5
	C2-C3	139,7	134,3
	N2-C3	141,2	139,1
	Si-X	225,0	227,2
	Si-Y	224,5	227,2
	N-Si-N	104,1	100,7
	X-Si-Y	87,3	88,0

Calculated at the B3LYP/cc-pVTZ level

Table S6-13. Calculated Wiberg-indices of the observed structures (B3LYP/cc-pVTZ)

H_2 (1)

	TS			product		
	Si-H	Si-H	H-H	Si-H	Si-H	H-H
A1	0.7076	0.7609	0.2399	0.9551	0.9551	0.0076
B1	0.6809	0.7037	0.2689	0.8434	0.8451	0.0004
C1	0.6832	0.6635	0.2687	0.9250	0.9249	0.0099
D1	0.7520	0.7254	0.2048	0.8682	0.8682	0.0288
E1	0.7345	0.7145	0.2174	0.8811	0.8810	0.0231
F1	0.7429	0.7384	0.2126	0.8732	0.8732	0.0055
G1	0.8013	0.6903	0.1750	0.8587	0.8587	0.0339

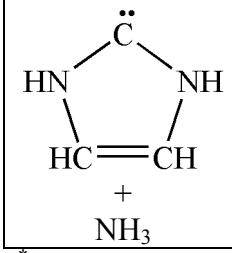
H_2O (2)

	TS			product		
H_2O	-	-	0.8018	-	-	-
A2	0.6168	0.5664	0.3027	0.6770	0.8970	0.0296
B2	0.6659	0.4819	0.2764	0.8432	0.6346	0.0243
C2	0.6026	0.4899	0.2993	0.8917	0.6452	0.0153
D2	0.6653	0.4797	0.2732	0.8573	0.6438	0.0281
E2	0.6549	0.4691	0.2755	0.8707	0.6325	0.0271
F2	0.6591	0.4900	0.2763	0.8610	0.6515	0.0279
G2	0.6643	0.4670	0.2679	0.8614	0.6405	0.0295

CH_3OH (3)

	TS			product		
	Si-H	Si-O	O-H	Si-H	Si-O	O-H
A3	0.6025	0.5466	0.2998	0.8974	0.6509	0.0293
B3	0.6560	0.4468	0.2726	0.8572	0.6127	0.0146
C3	0.5777	0.4597	0.3004	0.8872	0.6252	0.0155
D3	0.6498	0.4557	0.2705	0.8687	0.6242	0.0177
E3	0.6234	0.4511	0.2818	0.8829	0.6157	0.0167
F3	0.6382	0.4732	0.2759	0.8741	0.6361	0.0178
G3	0.6359	0.4507	0.2716	0.8716	0.6245	0.0189

NH_3 (4)

	TS			product		
	Si-H	Si-N	N-H	Si-H	Si-N	N-H
A4	0.6213	0.7090	0.3200	0.8873	0.7720	0.0414
B4	0.6501	0.6294	0.3000	0.8526	0.7290	0.0143
C4	0.5862	0.6439	0.3272	0.8707	0.7177	0.0372
D4	0.6326	0.6027	0.3127	0.8608	0.7490	0.0188
E4	0.6127	0.6224	0.3238	0.8752	0.7400	0.0164
F4	0.6403	0.6308	0.3096	0.8618	0.7622	0.0176
G4	0.6223	0.6084	0.3160	0.8578	0.7500	0.0208
	0.8032*	0.3797[i]	0.0772	0.9061*	1.0292[i]	0.0073

*Wiberg indices of the C-H bond
[i]Wiberg indices of the C-N bond

N_2H_4 (5)

	TS			product		
	Si-H	Si-N	N-H	Si-H	Si-N	N-H
A5	0.5500	0.7393	0.3507	0.8960	0.7472	0.0349
B5	0.6277	0.5780	0.2989	0.8592	0.6954	0.0170
C5	0.5395	0.6497	0.3503	0.8992	0.7062	0.0157
D5	0.5541	0.6627	0.3582	0.8557	0.7258	0.0232
E5	0.5737	0.6180	0.3375	0.8674	0.7178	0.0214
F5	0.5828	0.6418	0.3343	0.8576	0.7387	0.0228
G5	0.5391	0.6444	0.3501	0.8520	0.7287	0.0259

CH_3Cl (6)

	TS			product		
	Si-C	Si-Cl	C-Cl	Si-C	Si-Cl	C-Cl
A6	0.4266	0.6347	0.4989	0.8457	0.8381	0.0343
B6	0.4783	0.4161	0.4624	0.7725	0.7605	0.0339
C6	0.4117	0.5656	0.4695	0.7831	0.8199	0.0336
D6	0.4713	0.4326	0.4569	0.7899	0.7695	0.0416
E6	0.4618	0.4447	0.4630	0.8003	0.7692	0.0386
F6	0.4741	0.4711	0.4599	0.8012	0.7915	0.0398
G6	0.4586	0.3865	0.4449	0.8007	0.7585	0.0430

CH_3I (7)

	TS			product		
	Si-C	Si-I	C-I	Si-C	Si-I	C-I
A7	0.6025	0.5466	0.2998	0.8974	0.6509	0.0293
B7	0.4625	0.4107	0.5012	0.7718	0.8511	0.0372
C7	0.4025	0.6896	0.5130	0.7808	0.9606	0.0373
D7	0.4665	0.4082	0.4914	0.7902	0.8479	0.0493
E7	0.4618	0.4379	0.4997	0.8474	0.8003	0.0453
F7	0.4706	0.4884	0.4956	0.7995	0.8759	0.0478
G7	-	-	-	0.8017	0.8229	0.0509

P_4 (8)

	TS			product		
	Si-P	Si-P	P-P	Si-P	Si-P	P-P
A8	0.6794	0.6196	0.4929	0.9561	0.9561	0.0801
B8	0.6852	0.6405	0.4330	0.8524	0.8524	0.1145
C8	0.6879	0.6150	0.4977	0.9273	0.9273	0.0927
D8	0.6244	0.7520	0.3523	0.8627	0.8627	0.1276
E8	0.6285	0.7423	0.3699	0.8670	0.8673	0.1167
F8	0.7245	0.6852	0.3508	0.8754	0.8755	0.1247
G8	0.5665	0.7623	0.3120	0.8507	0.8507	0.1354

Table S14. Total energies of the observed structures (au) B3LYP/cc-pVTZ

1	-1.1799988	**A**	-290,6443319
2	-76,456199	**B**	-401,5203393
3	-115,7722495	**C**	-1609,6782067
4	-56,5847254	**D**	-478,9440132
5	-111.9158567	**E**	-499,7722238
6	-500.1644802	**F**	-555,1707509
7	-500.1644802	**G**	-477,7427727
8	-1365.580575		

Table S15-S16. Total energies of the observed structures (au) B3LYP/cc-pVTZ

Product

	1	**2**	**3**	**4**
A	-291.918335	-367.2210069	-406.5322297	-347.3280085
B	-402.7460139	-478.0619727	-517.3720193	-458.1658855
C	-1610.930935	-1686.240105	-1725.545734	-1666.343493
D	-480.1584288	-555.477832	-594.7880896	-535.5819599
E	-500.9924042	-576.3109065	-615.6207547	-556.4151208
F	-556.3871663	-631.707624	-671.0179103	-611.8126462
G	-478.9394269	-554.2616595	-593.571699	-534.3658102
	5	**6**	**7**	**8**
A	-402.6583395	-790.9525049	-626.5124415	-1656.29956030
B	-513.494789	-901.78989	-737.3473974	-1767.13799080
C	-1721.675111	-2109.964879	-1945.521514	-2975.31435600
D	-590.9112256	-979.204388	-814.7628277	-1844.55651500
E	-611.7439976	-1000.037481	-835.5960799	-1865.38797990
F	-667.1411673	-1055.432734	-890.9905939	-1920.69588370
G	-589.6944028	-977.9873258	-813.546556	-1843.34037500

TS

	1	**2**	**3**	**4**
A	-291.826217	-367.0967419	-406.4122525	-347.2145943
B	-402.6326401	-477.9375957	-517.2508269	-458.0459908
C	-1610.82835	-1686.117491	-1725.428411	-1666.231347
D	-480.043272	-555.3591327	-594.6727401	-535.4655539
E	-500.8850834	-576.189818	-615.5035426	-556.3001328
F	-556.2740784	-631.5864934	-670.9005678	-611.6955271
G	-478.8239237	-554.1456367	-593.4597075	-534.25237
	5	**6**	**7**	**8**
A	-402.5535792	-790.7734887	-626.3488336	-1656.23576680
B	-513.3804186	-901.6115404	-737.1865453	-1767.05089910
C	-1721.564551	-2109.790924	-1945.361551	-2975.23312700
D	-590.8023575	-979.0339996	-814.608606	-1844.46616400
E	-611.6331294	-999.8655868	-835.4403435	-1865.30525570
F	-667.0289828	-1055.260592	-890.8336507	-1920.783729
G	-589.592615	-977.8243493	-	-1843.25162100

Table S17-S18. Total Gibbs free energies of the observed structures (au)

B3LYP/cc-pVTZ

Product

	1	2	3	4
A	-291.908801	-367.207138	-406.493136	-347.302559
B	-402.70404	-478.014874	-517.300294	-458.107319
C	-1610.784148	-1686.088754	-1725.367621	-1666.179996
D	-480.08083	-555.395265	-594.680249	-535.488606
E	-500.921659	-576.234856	-615.519623	-556.329199
F	-556.303905	-631.617516	-670.902575	-611.711874
G	-478.886859	-554.202758	-593.487943	-534.296814
	5	**6**	**7**	**8**
A	-402.61765	-790.925308	-626.48809	-1656.306737
B	-513.420816	-901.73046	-737.290894	-1767.112425
C	-1721.495993	-2109.798837	-1945.35739	-2975.183751
D	-590.802152	-979.109449	-814.671292	-1844.49536
E	-611.641774	-999.94889	-835.510222	-1865.333415
F	-667.024652	-1055.329998	-890.890454	-1920.63078700
G	-589.609197	-977.915747	-813.477673	-1843.30293

TS

	1	2	3	4
A	-291.82114	-367.086855	-406.376732	-347.192397
B	-402.59438	-477.896614	-517.185424	-457.993931
C	-1610.685236	-1685.970115	-1725.254382	-1666.070336
D	-479.969595	-555.281339	-594.570062	-535.37648
E	-500.818763	-576.118674	-615.407126	-556.216545
F	-556.193145	-631.501045	-670.789995	-611.598078
G	-478.7755	-554.091683	-593.380409	-534.186421
	5	**6**	**7**	**8**
A	-402.515634	-790.751949	-626.329989	-1656.24673900
B	-513.312114	-901.558088	-737.135402	-1767.02976800
C	-1721.387423	-2109.628998	-1945.203148	-2975.10483200
D	-590.696569	-978.943943	-814.521546	-1844.40817200
E	-611.534483	-999.781593	-835.359189	-1865.25402000
F	-666.916341	-1055.162558	-890.739022	-1920.715005
G	-589.510055	-977.755878	-	-1843.21742200

Table S19. Total Gibbs free energies of the observed structures (au)

B3LYP/cc-pVTZ

	E	G
Arduengo carbene	-226,259465	-226,214422
Arduengo+NH_3 product	-282,8554170	-282,7734820
Arduengo + NH_3 TS	-282,7794497	-282,7068760

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
A	1	14	0.000000	0.000000	0.133135
	2	1	0.000000	1.093165	-0.931948
	3	1	0.000000	-1.093165	-0.931948
B	1	7	0.000000	1.326354	-0.442907
	2	14	0.000000	0.000000	0.665506
	3	7	0.000000	-1.326354	-0.442907
	4	1	0.000000	-1.288109	-1.452143
	5	1	0.000000	-2.275152	-0.106056
	6	1	0.000000	2.275152	-0.106056
	7	1	0.000000	1.288109	-1.452143
C	1	6	1.376795	-0.036850	-0.109199
	2	6	0.699086	-0.312721	-1.484320
	3	6	-0.699074	0.312687	-1.484323
	4	6	-1.376778	0.036841	-0.109196
	5	14	-2.765885	1.259952	0.279674
	6	14	2.765923	-1.259934	0.279675
	7	14	2.093491	1.731861	-0.012892
	8	14	0.000000	-0.000022	1.235135
	9	14	-2.093540	-1.731842	-0.012888
	10	1	1.059522	2.729920	0.385708
	11	1	3.191546	1.813150	0.980336
	12	1	2.598316	2.115809	-1.355262
	13	1	-3.912328	1.079291	-0.652855
	14	1	3.912371	-1.079243	-0.652843
	15	1	-2.598413	-2.115759	-1.355250
	16	1	-1.059595	-2.729948	0.385654
	17	1	-3.191574	-1.813097	0.980366
	18	1	3.262606	-1.087822	1.666473
	19	1	2.260414	-2.648194	0.110543
	20	1	-3.262583	1.087841	1.666466
	21	1	-2.260330	2.648193	0.110525
	22	1	-1.290041	-0.057669	-2.326074
	23	1	-0.608447	1.394486	-1.628678
	24	1	1.290052	0.057616	-2.326079
	25	1	0.608471	-1.394522	-1.628660
D	1	6	-1.234617	0.755431	0.140262
	2	6	-1.234619	-0.755429	-0.140262
	3	1	-1.957276	1.265469	-0.500098
	4	1	-1.957278	-1.265465	0.500098
	5	7	0.136181	1.209910	-0.115247
	6	1	0.293632	2.202707	-0.065366
	7	7	0.136179	-1.209910	0.115246
	8	1	0.293626	-2.202709	0.065371
	9	14	1.377256	-0.000001	0.000000
	10	1	-1.522692	0.945980	1.180961
	11	1	-1.522695	-0.945976	-1.180960

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
E	1	14	-1.532560	0.397922	0.000000
	2	7	0.000000	1.328050	0.000000
	3	6	1.284767	0.891405	0.000000
	4	6	1.621412	-0.431569	0.000000
	5	6	0.650321	-1.462420	0.000000
	6	6	-0.705339	-1.253853	0.000000
	7	1	-1.329661	-2.143050	0.000000
	8	1	-0.084160	2.334902	0.000000
	9	1	2.059112	1.649701	0.000000
	10	1	2.670301	-0.690020	0.000000
	11	1	1.033282	-2.480175	0.000000
F	1	6	2.407788	1.002072	0.000000
	2	6	1.204024	0.400455	0.000000
	3	7	0.000000	1.137075	0.000000
	4	14	-1.669278	0.650493	0.000000
	5	7	-1.364518	-1.076149	0.000000
	6	6	-0.121407	-1.697261	0.000000
	7	6	1.052893	-1.046054	0.000000
	8	1	-2.148992	-1.707908	0.000000
	9	1	-0.134515	-2.780071	0.000000
	10	1	1.960820	-1.630427	0.000000
	11	1	0.163849	2.134504	0.000000
	12	1	2.506586	2.078763	0.000000
	13	1	3.313981	0.416483	0.000000
G	1	6	-1.255113	-0.675546	-0.000003
	2	6	-1.255107	0.675556	0.000006
	3	1	-2.124213	-1.312805	-0.000008
	4	1	-2.124200	1.312823	-0.000001
	5	7	0.029138	-1.196362	-0.000009
	6	1	0.138368	-2.196735	0.000054
	7	7	0.029149	1.196360	0.000003
	8	1	0.138388	2.196731	-0.000012
	9	14	1.330355	-0.000004	0.000000

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
1	1	1	0.000000	0.000000	0.371478
	2	1	0.000000	0.000000	-0.371478
2	1	8	0.000000	0.000000	0.117614
	2	1	0.000000	0.760398	-0.470457
	3	1	0.000000	-0.760398	-0.470457
3	1	6	0.046384	0.662807	0.000000
	2	8	0.046384	-0.756841	0.000000
	3	1	-0.864448	-1.061424	0.000000
	4	1	-0.436565	1.080513	0.889726
	5	1	1.088198	0.978283	0.000000
	6	1	-0.436565	1.080513	-0.889726
4	1	7	0.000000	0.115430	0.000000
	2	1	-0.937980	-0.268925	0.000000
	3	1	0.468990	-0.269544	0.812153
	4	1	0.468990	-0.269544	-0.812153
5	1	1	1.140437	-0.307316	-0.786043
	2	7	-0.711000	-0.075861	-0.099609
	3	7	0.711002	-0.075703	0.099723
	4	1	-1.140602	-0.306069	0.786504
	5	1	-1.055900	0.836948	-0.380110
	6	1	1.056050	0.837387	0.378849
6	1	6	1.137768	0.000024	-0.000009
	2	1	1.477285	1.024312	-0.110742
	3	1	1.477278	-0.608143	-0.831628
	4	1	1.477303	-0.416289	0.942406
	5	17	-0.662263	-0.000001	0.000001
7	1	6	-1.833534	0.000000	-0.000011
	2	53	0.329623	0.000000	-0.000001
	3	1	-2.156194	-0.008288	1.033625
	4	1	-2.156328	-0.891015	-0.523942
	5	1	-2.156285	0.899318	-0.509579
8	1	15	0.710140	-0.924154	-0.691930
	2	15	-1.296384	-0.388790	0.073850
	3	15	0.077615	1.196119	-0.632769
	4	15	0.508628	0.116825	1.250849

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-A1	1	14	-0,000001	0,000003	-0,000014
	2	1	-1,071036	0,375500	-0,953382
	3	1	1,085637	-0,700143	-0,726884
	4	1	-0,556837	-0,897348	1,040139
	5	1	0,542249	1,221946	0,640322
Pr-B1	1	14	-0,000006	0,502189	-0,000001
	2	7	1,396938	-0,506193	-0,001125
	3	1	1,562039	-1,172821	-0,737952
	4	1	2,258435	-0,180803	0,405575
	5	7	-1,396931	-0,506255	0,001069
	6	1	-2,258569	-0,180579	-0,405121
	7	1	-1,561872	-1,172921	0,737904
	8	1	0,209089	1,381802	1,185410
	9	1	-0,209096	1,381814	-1,185401
Pr-C1	1	6	-1,436073	-0,021164	0,096782
	2	6	-0,699819	-0,320910	1,449608
	3	6	0,699995	0,320296	1,449553
	4	6	1,436090	0,020852	0,096514
	5	14	2,698965	1,370446	-0,302287
	6	14	-2,700325	-1,369510	-0,301958
	7	14	-2,295884	1,666934	0,139320
	8	14	-0,000118	-0,001005	-1,156300
	9	14	2,297280	-1,666512	0,139334
	10	1	-1,321360	2,766007	0,367141
	11	1	-2,996021	1,925867	-1,143543
	12	1	-3,288604	1,699552	1,246270
	13	1	3,792311	1,389603	0,706361
	14	1	-3,796284	-1,384666	0,703936
	15	1	3,293566	-1,696628	1,243163
	16	1	1,324016	-2,765612	0,372403
	17	1	2,993468	-1,927461	-1,145251
	18	1	-3,301489	-1,153471	-1,642542
	19	1	-2,034000	-2,697623	-0,279564
	20	1	3,303793	1,152442	-1,640917
	21	1	2,030488	2,697546	-0,284501
	22	1	1,278018	-0,033034	2,307457
	23	1	0,591099	1,400364	1,581557
	24	1	-1,277678	0,032252	2,307689
	25	1	-0,590889	-1,401001	1,581286
	26	1	-0,033310	1,192287	-2,045619
	27	1	0,032859	-1,195825	-2,043605

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-D1	1	6	1,287166	-0,745646	0,178295
	2	6	1,287292	0,745558	-0,178175
	3	7	-0,043934	1,249288	0,185847
	4	14	-1,234464	0,000036	0,000058
	5	7	-0,043995	-1,249262	-0,186191
	6	1	-2,134343	0,120279	-1,183528
	7	1	-0,208791	-2,216137	0,038666
	8	1	-0,208583	2,216210	-0,038870
	9	1	2,069744	1,267426	0,377442
	10	1	2,069744	-1,267598	-0,377061
	11	1	1,498897	0,864369	-1,248440
	12	1	1,498416	-0,864470	1,248632
	13	1	-2,133836	-0,120244	1,184039
Pr-E1	1	6	0,250451	1,459427	-0,000142
	2	14	1,424282	0,039565	0,000166
	3	7	0,305469	-1,327047	-0,000438
	4	6	-1,062433	-1,212435	-0,000020
	5	6	-1,737456	-0,039422	0,000341
	6	6	-1,086801	1,245592	-0,000087
	7	1	0,644694	-2,274956	0,000010
	8	1	-1,606773	-2,148832	-0,000013
	9	1	-2,816429	-0,075654	0,000312
	10	1	-1,748632	2,107417	-0,000348
	11	1	0,603809	2,483829	-0,000805
	12	1	2,331691	-0,037870	-1,182352
	13	1	2,330832	-0,037480	1,183398
Pr-F1	1	6	2,625288	-0,445201	0,000031
	2	6	1,317887	-0,123891	0,000000
	3	7	0,316345	-1,112550	-0,000179
	4	14	-1,394885	-0,880457	0,000117
	5	7	-1,524570	0,853156	-0,000159
	6	6	-0,406123	1,676787	-0,000027
	7	6	0,872313	1,262761	0,000086
	8	1	-2,055405	-1,481907	1,190629
	9	1	-2,055741	-1,482402	-1,189952
	10	1	0,686855	-2,050031	-0,000480
	11	1	1,646060	2,014960	0,000219
	12	1	-0,621293	2,737639	-0,000001
	13	1	-2,410116	1,327481	-0,000291
	14	1	3,378284	0,326860	0,000095
	15	1	2,961129	-1,473185	-0,000029

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-G1	1	6	1,330810	-0,668990	0,000035
	2	7	0,036571	-1,238103	0,000124
	3	14	-1,184824	0,000000	0,000003
	4	7	0,036556	1,238105	-0,000173
	5	6	1,330813	0,668990	-0,000021
	6	1	-0,055729	-2,235831	-0,000440
	7	1	-0,055722	2,235833	0,000611
	8	1	2,200656	1,303453	-0,000042
	9	1	2,200669	-1,303434	0,000040
	10	1	-2,091961	0,000218	1,186064
Pr-A2	1	14	-0.535464	-0.008916	0.000000
	2	1	-1.034424	1.382667	-0.000010
	3	8	1.121303	0.111590	0.000000
	4	1	-1.036348	-0.725716	1.202455
	5	1	-1.036346	-0.725732	-1.202446
	6	1	1.633194	-0.699114	0.000000
Pr-B2	1	7	1.622958	-0.195336	-0.211551
	2	14	0.000893	-0.079862	0.342676
	3	8	-1.121574	-1.181298	-0.195371
	4	7	-0.535657	1.471635	-0.182764
	5	1	0.055757	2.276233	-0.049096
	6	1	-1.508523	1.720134	-0.100912
	7	1	2.242550	-0.893414	0.166570
	8	1	1.871240	0.043422	-1.158361
	9	1	0.044172	-0.372412	1.792808
	10	1	-1.356225	-1.139600	-1.125293

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-C2	1	6	1.435172	0.118058	0.213542
	2	14	0.004056	-0.199829	-0.998401
	3	8	-0.031559	-1.712945	-1.689305
	4	14	2.250847	1.787943	-0.167075
	5	14	2.747741	-1.241234	0.163973
	6	6	0.709633	0.146847	1.602826
	7	6	-0.690494	0.771090	1.453765
	8	6	-1.423500	0.165601	0.206615
	9	14	-2.658906	1.399654	-0.523541
	10	14	-2.344296	-1.425911	0.664221
	11	1	1.288982	0.691575	2.352315
	12	1	-0.580114	1.851886	1.330475
	13	1	-3.773539	1.656329	0.428149
	14	1	-1.973428	2.691668	-0.786615
	15	1	-3.235554	0.888910	-1.792034
	16	1	-3.198324	-1.896525	-0.452927
	17	1	-1.401958	-2.526325	1.013337
	18	1	-3.196158	-1.178379	1.856496
	19	1	2.979441	1.730719	-1.458289
	20	1	1.244802	2.879041	-0.249709
	21	1	3.209730	2.133766	0.915743
	22	1	3.429333	-1.298644	-1.152045
	23	1	3.770451	-1.016996	1.219843
	24	1	2.112011	-2.560708	0.432643
	25	1	0.029778	0.689245	-2.184331
	26	1	0.035209	-2.487303	-1.125836
	27	1	-1.267490	0.629165	2.370795
	28	1	0.602230	-0.872146	1.987471
Pr-D2	1	6	-1.562257	0.776982	0.359467
	2	7	-0.333154	1.231007	-0.298459
	3	14	0.835429	-0.035427	-0.414826
	4	8	2.185309	0.034745	0.545584
	5	6	-1.676846	-0.722273	0.044805
	6	7	-0.306370	-1.245098	0.063128
	7	1	-2.436884	1.310709	-0.018236
	8	1	-2.301886	-1.219197	0.790223
	9	1	-0.121015	2.209848	-0.210531
	10	1	-0.215747	-2.223455	-0.153714
	11	1	-1.528451	0.921685	1.447266
	12	1	-2.155047	-0.853657	-0.933891
	13	1	1.457173	-0.153521	-1.750109
	14	1	2.034651	-0.004013	1.493573

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-E2	1	6	0.111643	1.447025	-0.244658
	2	14	-1.051206	0.039378	-0.403276
	3	8	-2.270128	-0.018020	0.726327
	4	6	1.413081	1.241396	0.088879
	5	6	2.037833	-0.036290	0.279177
	6	6	1.385382	-1.212107	0.103994
	7	7	0.066945	-1.315799	-0.253053
	8	1	-0.221063	2.470602	-0.374476
	9	1	-0.261384	-2.261095	-0.373748
	10	1	1.912225	-2.148983	0.237897
	11	1	3.081273	-0.071248	0.554628
	12	1	2.059754	2.105339	0.217073
	13	1	-1.826854	-0.102468	-1.654074
	14	1	-2.022284	0.171176	1.634960
Pr-F2	1	6	2.668784	-1.114393	0.106929
	2	6	1.530721	-0.401377	0.011694
	3	6	1.516455	1.045643	0.172243
	4	6	0.425901	1.827728	0.108708
	5	7	-0.871746	1.384811	-0.117806
	6	14	-1.261853	-0.283742	-0.387089
	7	8	-2.388213	-0.881672	0.663631
	8	7	0.291059	-1.016991	-0.248503
	9	1	-2.167402	-0.870423	1.598738
	10	1	2.681435	-2.188625	-0.016532
	11	1	3.606750	-0.622660	0.310780
	12	1	2.468685	1.519499	0.355090
	13	1	0.529620	2.897137	0.240375
	14	1	-1.572661	2.104466	-0.155361
	15	1	0.365325	-2.015252	-0.374028
	16	1	-1.926457	-0.518731	-1.682143
Pr-G2	1	6	1.655330	-0.669925	-0.218750
	2	7	0.409650	-1.230309	0.134891
	3	14	-0.783645	-0.000156	0.410271
	4	8	-2.108813	0.000081	-0.583053
	5	6	1.655206	0.670172	-0.218626
	6	7	0.409446	1.230269	0.135145
	7	1	2.487107	-1.304288	-0.473974
	8	1	2.486875	1.304721	-0.473746
	9	1	0.326217	-2.227330	0.200526
	10	1	0.325781	2.227269	0.200799
	11	1	-1.445009	-0.000547	1.729630
	12	1	-1.936324	0.000516	-1.528599

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-A3	1	6	-1.647854	0.204732	-0.000004
	2	8	-0.455411	-0.564320	0.000029
	3	14	1.063291	0.090174	-0.000001
	4	1	2.004445	-1.049838	-0.001107
	5	1	1.282084	0.938025	1.203694
	6	1	1.281254	0.939639	-1.202715
	7	1	-1.714841	0.840070	-0.888393
	8	1	-2.492696	-0.482583	-0.001147
	9	1	-1.715907	0.838422	0.889478
Pr-B3	1	7	1.301232	-1.247622	-0.420799
	2	14	0.513718	0.004015	0.453678
	3	7	0.878889	1.449939	-0.410981
	4	8	-1.133579	-0.061957	0.612343
	5	1	1.823878	1.631415	-0.708939
	6	1	0.401514	2.306453	-0.179806
	7	1	1.464343	-2.149303	-0.004143
	8	1	1.252323	-1.304112	-1.425031
	9	1	0.966324	-0.112646	1.857639
	10	6	-2.057499	-0.141790	-0.458719
	11	1	-3.064585	-0.120100	-0.042553
	12	1	-1.947778	0.695744	-1.153104
	13	1	-1.935292	-1.073482	-1.019531

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-C3	1	6	-1.422768	-0.394068	0.212922
	2	14	-2.404824	0.989068	1.053113
	3	6	-0.692544	-1.265288	1.295209
	4	6	0.702453	-0.684017	1.590408
	5	6	1.432935	-0.340992	0.248003
	6	14	2.225676	-1.897968	-0.503474
	7	14	0.008231	0.218967	-0.889030
	8	8	-0.024231	1.792622	-1.380052
	9	6	-0.024608	3.045255	-0.715031
	10	14	-2.627214	-1.454532	-0.795554
	11	14	2.812841	0.924779	0.505261
	12	1	-1.274564	-1.338549	2.217790
	13	1	1.279150	-1.382213	2.202544
	14	1	3.098545	-2.543432	0.512198
	15	1	1.207261	-2.891637	-0.930481
	16	1	3.044898	-1.539092	-1.688299
	17	1	3.303492	1.464183	-0.786915
	18	1	2.321132	2.050770	1.342677
	19	1	3.964597	0.309241	1.218197
	20	1	-3.255692	-0.660282	-1.881236
	21	1	-1.903598	-2.606275	-1.392797
	22	1	-3.706108	-1.991700	0.076405
	23	1	-3.074031	1.864379	0.058928
	24	1	-3.442233	0.392341	1.935035
	25	1	-1.531703	1.838024	1.906767
	26	1	0.044790	-0.489828	-2.191537
	27	1	0.317138	2.972754	0.318507
	28	1	0.642335	3.719595	-1.252532
	29	1	-1.029906	3.469186	-0.722337
	30	1	0.586362	0.222819	2.190502
	31	1	-0.576750	-2.291003	0.933510
Pr-D3	1	6	-1.695497	0.921523	0.468064
	2	6	-1.945857	-0.593812	0.510024
	3	7	-0.654031	-1.228520	0.225367
	4	14	0.327884	-0.232008	-0.794740
	5	8	1.899697	-0.098166	-0.304159
	6	7	-0.707438	1.135789	-0.593807
	7	1	-2.626701	1.452251	0.258648
	8	1	-2.326147	-0.887282	1.491221
	9	1	-0.457367	2.091591	-0.779276
	10	1	-0.670780	-2.233567	0.181262
	11	1	-1.331910	1.260854	1.446578
	12	1	-2.706111	-0.857940	-0.235626
	13	1	0.513473	-0.657926	-2.197187
	14	6	2.314327	0.252079	1.007523
	15	1	3.398493	0.155375	1.057112
	16	1	2.046266	1.285315	1.246076
	17	1	1.865281	-0.404860	1.756238

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
PrE3	1	6	0.472033	1.431544	-0.450601
	2	14	-0.592740	-0.000363	-0.875630
	3	8	-2.064256	-0.060564	-0.117450
	4	6	-2.271788	0.082511	1.280159
	5	6	1.631570	1.258618	0.236075
	6	6	2.186435	-0.002395	0.639279
	7	6	1.620994	-1.193836	0.324710
	8	7	0.456430	-1.330992	-0.384913
	9	1	0.184922	2.444518	-0.709063
	10	1	0.190533	-2.284977	-0.572093
	11	1	2.098642	-2.117154	0.629118
	12	1	3.110616	-0.011310	1.197633
	13	1	2.214914	2.136168	0.502194
	14	1	-0.997971	-0.175732	-2.286418
	15	1	-3.342020	0.189346	1.453682
	16	1	-1.916015	-0.797146	1.823380
	17	1	-1.761706	0.964174	1.676653
Pr-F3	1	6	2.714549	-1.442923	0.173221
	2	6	1.719073	-0.547495	0.031221
	3	7	0.494819	-0.891187	-0.573956
	4	14	-0.892680	0.100189	-0.828431
	5	8	-2.265973	-0.477204	-0.129146
	6	6	1.852351	0.826915	0.492855
	7	6	0.909300	1.778786	0.394591
	8	7	-0.354395	1.608124	-0.158018
	9	6	-2.420564	-0.786889	1.251245
	10	1	2.618708	-2.462574	-0.174060
	11	1	3.643754	-1.158596	0.641065
	12	1	2.794685	1.093513	0.946357
	13	1	1.116944	2.773756	0.767126
	14	1	-0.927154	2.433825	-0.185104
	15	1	0.471321	-1.845724	-0.899600
	16	1	-1.304421	0.207813	-2.239860
	17	1	-3.405187	-1.231795	1.386547
	18	1	-1.661724	-1.497186	1.586803
	19	1	-2.352842	0.113035	1.866951

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center Number	Atomic Number	X	Y	Z
Pr-G3	1	6	1.835359	0.670279	0.553529
	2	6	1.835441	-0.669679	0.554090
	3	7	0.771924	-1.231203	-0.184454
	4	14	-0.270755	-0.000409	-0.828338
	5	8	-1.833689	-0.000278	-0.299337
	6	7	0.771798	1.231051	-0.185526
	7	1	2.538262	1.304550	1.066556
	8	1	2.538423	-1.303429	1.067652
	9	1	0.726755	2.227036	-0.291359
	10	1	0.726996	-2.227282	-0.289446
	11	1	-0.480091	-0.001051	-2.288840
	12	6	-2.230209	0.000548	1.066318
	13	1	-3.318883	0.000672	1.100413
	14	1	-1.860576	-0.886108	1.586854
	15	1	-1.860403	0.887727	1.585839
Pr-A4	1	7	1.153155	0.000000	-0.065767
	2	14	-0.577605	0.000000	0.003559
	3	1	-1.060134	-1.218366	-0.692509
	4	1	-1.060132	1.218375	-0.692495
	5	1	-1.181931	-0.000007	1.368264
	6	1	1.658288	0.826567	0.213639
	7	1	1.658288	-0.826567	0.213642
Pr-B4	1	7	1.529107	-0.677100	-0.228467
	2	14	-0.000347	-0.080811	0.332756
	3	7	-1.530693	-0.673753	-0.228906
	4	1	-1.787807	-0.585264	-1.205229
	5	1	-1.904769	-1.526187	0.170139
	6	1	1.786106	-0.589686	-1.204928
	7	1	1.900820	-1.530524	0.170683
	8	1	-0.001340	-0.458052	1.776306
	9	7	0.002105	1.574417	-0.157290
	10	1	-0.833611	2.130579	-0.029296
	11	1	0.841822	2.125546	-0.033620

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
	Number	Number	X	Y	Z
Pr-C4	1	6	-1.428557	0.137222	-0.223704
	2	14	-2.320790	1.746564	0.225163
	3	14	-2.677961	-1.279952	-0.245264
	4	6	-0.708966	0.265764	-1.609203
	5	6	0.690755	0.881282	-1.421587
	6	6	1.422867	0.190478	-0.223757
	7	14	2.263883	-1.418034	-0.765382
	8	14	0.004181	-0.169568	1.002210
	9	7	0.030130	-1.711262	1.769579
	10	14	2.722923	1.330376	0.538237
	11	1	-0.600365	-0.722738	-2.066346
	12	1	1.264704	0.805683	-2.348494
	13	1	3.870406	1.535627	-0.387542
	14	1	2.117677	2.658658	0.819399
	15	1	3.251339	0.764538	1.805751
	16	1	3.169129	-1.936536	0.289732
	17	1	1.278353	-2.487384	-1.085250
	18	1	3.058980	-1.166201	-1.996371
	19	1	-2.971619	1.635180	1.554654
	20	1	-1.376202	2.894253	0.266315
	21	1	-3.361348	2.054286	-0.792715
	22	1	-3.382765	-1.416609	1.053241
	23	1	-3.695901	-1.049967	-1.306052
	24	1	-1.992424	-2.561869	-0.561189
	25	1	-0.017230	0.784384	2.144650
	26	1	0.119190	-1.805842	2.766067
	27	1	0.021835	-2.597723	1.295443
	28	1	-1.290295	0.861006	-2.317979
	29	1	0.577722	1.950213	-1.220363

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center Number	Atomic Number	X	Y	Z
Pr-D4	1	6	-1.698782	-0.735063	0.035715
	2	7	-0.323246	-1.234367	0.062091
	3	14	0.811017	-0.016533	-0.417021
	4	7	2.227387	-0.014195	0.551980
	5	6	-1.604695	0.759952	0.375137
	6	7	-0.381402	1.238495	-0.273429
	7	1	-2.324207	-1.251711	0.767692
	8	1	-2.487177	1.288746	0.007015
	9	1	-0.210300	-2.217057	-0.120395
	10	1	-0.160107	2.207485	-0.118855
	11	1	-2.168557	-0.856572	-0.949242
	12	1	-1.573569	0.883833	1.466011
	13	1	1.378097	-0.080659	-1.790460
	14	1	3.133017	0.195599	0.168737
	15	1	2.220260	-0.017063	1.558185
Pr-E4	1	6	-0.148508	1.442442	-0.210266
	2	6	-1.453992	1.237369	0.103200
	3	6	-2.084234	-0.041406	0.266315
	4	6	-1.420107	-1.213525	0.111739
	5	7	-0.095176	-1.312352	-0.216912
	6	14	1.025624	0.044647	-0.410129
	7	1	0.192494	2.467710	-0.303440
	8	1	0.247586	-2.257737	-0.285362
	9	1	-1.942048	-2.152882	0.249870
	10	1	-3.132573	-0.080225	0.522119
	11	1	-2.097016	2.102092	0.245590
	12	1	1.721113	-0.082168	-1.719751
	13	7	2.342977	-0.006539	0.693375
	14	1	2.262307	0.180109	1.678668
	15	1	3.295827	-0.119000	0.392931
Pr-F4	1	6	2.640386	-1.233536	-0.080341
	2	6	1.537273	-0.462530	-0.017661
	3	6	1.607264	0.986855	-0.134923
	4	6	0.551520	1.818892	-0.120247
	5	7	-0.773262	1.434934	0.030843
	6	14	-1.248159	-0.201540	0.389937
	7	7	-2.508421	-0.830965	-0.575907
	8	7	0.254335	-1.015995	0.140411
	9	1	-1.800475	-0.315848	1.763729
	10	1	0.259065	-2.023763	0.181372
	11	1	2.590301	1.416166	-0.253564
	12	1	0.713086	2.883613	-0.233480
	13	1	-1.442529	2.184960	0.024755
	14	1	3.611410	-0.788783	-0.230642
	15	1	2.589415	-2.310085	0.009210
	16	1	-2.471830	-0.913327	-1.577975
	17	1	-3.401445	-1.085274	-0.190925

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-G4	1	6	1.693370	0.671960	-0.217590
	2	7	0.441173	1.226184	0.116384
	3	14	-0.756780	-0.002346	0.409023
	4	7	-2.156231	0.004093	-0.577287
	5	6	1.695221	-0.668260	-0.219800
	6	7	0.444592	-1.227059	0.112312
	7	1	2.528835	1.309003	-0.453862
	8	1	2.532511	-1.302153	-0.458118
	9	1	0.338517	2.223422	0.127914
	10	1	0.345833	-2.224692	0.123869
	11	1	-1.357170	-0.008612	1.769815
	12	1	-3.083692	-0.013154	-0.188088
	13	1	-2.148202	0.004308	-1.583381
Pr-A5	1	14	-1.080286	-0.107623	-0.000521
	2	1	-2.001166	1.059157	0.009316
	3	7	0.515536	0.559553	-0.053391
	4	1	-1.332406	-0.952142	-1.193046
	5	1	-1.352163	-0.940851	1.204924
	6	7	1.593692	-0.368253	-0.014178
	7	1	2.041121	-0.372703	0.896126
	8	1	0.718561	1.493345	0.273811
	9	1	2.285450	-0.119191	-0.710852
Pr-B5	1	7	1.140897	1.489616	-0.223091
	2	14	0.416956	0.025276	0.338143
	3	7	1.493694	-1.229964	-0.159439
	4	1	1.359572	1.630686	-1.196678
	5	1	0.919201	2.360096	0.231994
	6	1	1.261505	-2.194763	0.011962
	7	1	2.486197	-1.075654	-0.088373
	8	1	0.196156	0.274620	1.783080
	9	7	-1.106119	-0.528925	-0.280919
	10	7	-2.281463	0.181681	0.094506
	11	1	-3.013668	-0.474246	0.338422
	12	1	-1.158702	-1.020791	-1.163065
	13	1	-2.616707	0.759326	-0.668728

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-C5	1	6	-1.335774	-0.576624	0.234863
	2	14	-2.255779	0.526179	1.464937
	3	14	-0.010896	0.440555	-0.700053
	4	7	-0.080670	2.167379	-0.556184
	5	7	-0.984648	2.862930	-1.408469
	6	6	-0.491312	-1.665787	0.980630
	7	6	0.881511	-1.094230	1.381938
	8	6	1.507955	-0.298641	0.185639
	9	14	2.737783	0.991033	0.810785
	10	14	-2.576384	-1.384021	-0.939984
	11	14	2.413532	-1.465948	-1.005789
	12	1	-1.326151	1.197833	2.413036
	13	1	-3.034493	1.583136	0.768505
	14	1	-3.200472	-0.288039	2.276104
	15	1	3.793095	0.340294	1.632555
	16	1	-3.525784	-2.252054	-0.191135
	17	1	3.509669	-2.167800	-0.284698
	18	1	1.498295	-2.499512	-1.555753
	19	1	2.995232	-0.708795	-2.141597
	20	1	-3.362238	-0.362301	-1.676623
	21	1	-1.856512	-2.239668	-1.919233
	22	1	3.393129	1.718286	-0.303780
	23	1	2.049159	1.980107	1.685506
	24	1	1.539371	-1.897706	1.723424
	25	1	0.748400	-0.429542	2.240639
	26	1	-1.011811	-2.051950	1.861209
	27	1	-0.332982	-2.526373	0.324608
	28	1	-0.041287	0.165100	-2.157442
	29	1	-0.509582	3.643374	-1.845574
	30	1	0.218164	2.667706	0.269021
	31	1	-1.775848	3.218257	-0.883156
Pr-D5	1	6	-1.692493	1.028419	0.283695
	2	7	-0.685176	1.021054	-0.783628
	3	14	0.302675	-0.397654	-0.698211
	4	7	-0.759103	-1.172888	0.431374
	5	6	-2.022497	-0.444261	0.566551
	6	1	0.498506	-1.118005	-1.986634
	7	1	-0.299391	1.924385	-1.003387
	8	1	-0.822267	-2.169968	0.549836
	9	1	-2.441193	-0.549791	1.570648
	10	1	-2.593995	1.565740	-0.020514
	11	1	-2.779219	-0.793028	-0.148335
	12	1	-1.311237	1.497432	1.198790
	13	7	1.945633	-0.168825	-0.228884
	14	7	2.280091	0.505525	0.975221
	15	1	2.981730	1.212672	0.791625
	16	1	2.697056	-0.657624	-0.696315
	17	1	2.652391	-0.143658	1.659183

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-E5	1	6	-0.522038	1.436097	-0.385442
	2	6	-1.705406	1.246296	0.251879
	3	6	-2.271191	-0.025160	0.602780
	4	6	-1.673631	-1.204520	0.304524
	5	7	-0.481959	-1.319845	-0.360970
	6	14	0.560121	0.023815	-0.834083
	7	1	-0.173767	-2.268727	-0.502564
	8	1	-2.143675	-2.137348	0.591918
	9	1	-3.216211	-0.051674	1.124634
	10	1	-2.294204	2.117428	0.527441
	11	1	-0.217454	2.456574	-0.590436
	12	1	0.940558	-0.102253	-2.269836
	13	7	2.128032	-0.059710	-0.114599
	14	7	2.308388	0.073087	1.286642
	15	1	2.832141	0.913643	1.501573
	16	1	2.966226	-0.108920	-0.677481
	17	1	2.817064	-0.723140	1.651963
Pr-F5	1	6	-2.738128	-1.491371	0.193386
	2	6	-1.758001	-0.578274	0.047600
	3	6	-1.938716	0.809415	0.447809
	4	6	-1.004455	1.771162	0.360081
	5	7	0.277342	1.604645	-0.143898
	6	14	0.855116	0.101687	-0.792050
	7	7	-0.505734	-0.916791	-0.493787
	8	1	1.219459	0.195113	-2.229937
	9	7	2.345650	-0.433786	-0.128657
	10	1	-0.434447	-1.892086	-0.740436
	11	1	-2.903248	1.074198	0.853157
	12	1	-1.238700	2.772480	0.699044
	13	1	0.864708	2.419162	-0.106869
	14	1	-3.687220	-1.211985	0.622837
	15	1	-2.606753	-2.522027	-0.106938
	16	7	2.503319	-0.670051	1.261269
	17	1	3.267295	-0.114696	1.627076
	18	1	3.134774	-0.649807	-0.722357
	19	1	2.704271	-1.647685	1.435393
	10	7	3.635600	1.074908	0.182494
	11	1	3.394959	-1.279771	0.805772
	12	7	3.276442	2.406677	-0.148561
	13	1	3.614213	2.642607	-1.074194
	14	1	4.624385	0.860188	0.195935
	15	1	3.682806	3.056047	0.514566

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-F6	1	6	-0.074471	-0.203102	-0.016972
	2	6	-0.018188	0.134424	1.278434
	3	7	1.295699	0.176136	1.787909
	4	14	2.472727	-0.140186	0.548894
	5	7	1.192733	-0.442574	-0.587003
	6	1	1.252756	-0.637345	-1.568573
	7	1	1.439610	0.483976	2.731068
	8	1	-0.858220	0.365540	1.911338
	9	1	-0.967653	-0.291962	-0.611891
	10	7	3.635600	1.074908	0.182494
	11	1	3.394959	-1.279771	0.805772
	12	7	3.276442	2.406677	-0.148561
	13	1	3.614213	2.642607	-1.074194
Pr-F6	1	6	-0.074471	-0.203102	-0.016972
	2	6	-0.018188	0.134424	1.278434
	3	7	1.295699	0.176136	1.787909
	4	14	2.472727	-0.140186	0.548894
	5	7	1.192733	-0.442574	-0.587003
	6	1	1.252756	-0.637345	-1.568573
	7	1	1.439610	0.483976	2.731068
	8	1	-0.858220	0.365540	1.911338
	9	1	-0.967653	-0.291962	-0.611891
	10	7	3.635600	1.074908	0.182494
	11	1	3.394959	-1.279771	0.805772
	12	7	3.276442	2.406677	-0.148561
	13	1	3.614213	2.642607	-1.074194
	14	1	4.624385	0.860188	0.195935
	15	1	3.682806	3.056047	0.514566
Pr-A7	1	6	2,608131	-0,830543	0,000000
	2	14	1,467194	0,656412	0,000000
	3	53	-0,906551	-0,071716	0,000000
	4	1	3,647274	-0,493601	-0,000111
	5	1	2,446097	-1,446867	-0,883812
	6	1	2,446247	-1,446749	0,883922
	7	1	1,659030	1,490830	1,208888
	8	1	1,659032	1,490831	-1,208887

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-B7	1	6	1,784049	1,670282	-0,601474
	2	14	1,262641	-0,033944	-0,024936
	3	7	2,027920	-0,332549	1,481405
	4	53	-1,264087	0,010949	0,033216
	5	7	1,601964	-1,382174	-1,025997
	6	1	2,868315	1,706124	-0,728066
	7	1	1,494869	2,438423	0,116942
	8	1	1,316425	1,912182	-1,555195
	9	1	0,979928	-1,671369	-1,760578
	10	1	2,127112	0,412556	2,153225
	11	1	1,873388	-1,215223	1,944161
	12	1	2,546127	-1,706425	-1,160852
Pr-C7	1	6	0,314724	-0,091550	2,440854
	2	14	0,182055	-0,018101	0,564933
	3	53	-2,316355	-0,033739	0,186036
	4	6	1,059484	-1,417664	-0,381208
	5	14	2,519095	-2,112272	0,626067
	6	6	1,582931	-0,657446	-1,644381
	7	6	2,090951	0,736731	-1,239712
	8	6	1,039595	1,450216	-0,310569
	9	14	-0,087028	2,532982	-1,396910
	10	14	-0,014126	-2,905281	-0,871788
	11	14	1,926302	2,602860	0,907544
	12	1	3,319110	-1,045187	1,281268
	13	1	2,027005	-3,028292	1,685161
	14	1	3,419954	-2,861035	-0,286771
	15	1	2,673487	3,649168	0,163336
	16	1	0,868458	-3,995391	-1,372028
	17	1	0,774289	3,562012	-2,040296
	18	1	-0,721505	1,737170	-2,475245
	19	1	-1,127881	3,223656	-0,601530
	20	1	-0,771078	-3,428126	0,290649
	21	1	-0,944510	-2,529767	-1,962690
	22	1	0,961283	3,267750	1,819174
	23	1	2,905834	1,838004	1,722064
	24	1	2,305004	1,332471	-2,130559
	25	1	3,046249	0,627905	-0,717863
	26	1	2,373517	-1,215170	-2,152605
	27	1	0,771226	-0,544597	-2,368094
	28	1	-0,152085	-1,005416	2,809173
	29	1	1,352431	-0,072696	2,776717
	30	1	-0,208258	0,751325	2,892477

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-D7	1	6	0,476876	2,498632	0,118418
	2	14	0,731988	0,650891	0,026667
	3	53	-1,619059	-0,306221	-0,026205
	4	7	1,725739	-0,029397	1,266347
	5	6	2,520694	-1,136088	0,708335
	6	6	2,852321	-0,741157	-0,741090
	7	7	1,703608	0,022941	-1,234698
	8	1	1,605315	0,140055	-2,225843
	9	1	1,383811	-0,192005	2,199767
	10	1	3,437299	-1,281304	1,282416
	11	1	3,768288	-0,139301	-0,762193
	12	1	1,964112	-2,080701	0,715389
	13	1	3,025126	-1,635063	-1,343159
	14	1	-0,096211	2,764842	1,006855
	15	1	1,444722	3,000493	0,157500
	16	1	-0,074962	2,857103	-0,750711
Pr-E7	1	6	-1,566816	0,135353	1,466488
	2	6	-2,654155	-0,637501	1,214414
	3	6	-3,139119	-1,006101	-0,085528
	4	6	-2,581920	-0,564786	-1,238727
	5	7	-1,502306	0,280654	-1,300168
	6	14	-0,536930	0,753196	0,086974
	7	1	-1,198614	0,506326	-2,234376
	8	1	-2,996766	-0,863859	-2,192923
	9	1	-3,998501	-1,655838	-0,154954
	10	1	-3,223829	-1,018893	2,057031
	11	1	-1,299167	0,327079	2,498393
	12	53	1,719200	-0,408504	-0,007426
	13	6	-0,109375	2,574638	0,021355
	14	1	0,513310	2,847411	0,873773
	15	1	0,448227	2,815472	-0,884312
	16	1	-1,020811	3,174096	0,046480

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-F7	1	6	-0,323931	2,234412	-1,416923
	2	14	0,235412	0,825221	-0,331756
	3	53	-1,845933	-0,516260	0,150465
	4	7	0,974955	1,324599	1,151468
	5	6	2,102968	0,675514	1,648233
	6	6	2,836000	-0,231249	0,981964
	7	6	2,581577	-0,702154	-0,372306
	8	7	1,480093	-0,126178	-1,039887
	9	6	3,367092	-1,616948	-0,967999
	10	1	0,480047	1,891426	1,818776
	11	1	2,384944	0,955592	2,654633
	12	1	3,692618	-0,654089	1,484081
	13	1	1,337404	-0,502668	-1,964972
	14	1	3,175067	-1,967369	-1,972671
	15	1	4,222016	-2,022754	-0,450745
	16	1	-1,091145	2,826623	-0,917594
	17	1	0,524183	2,877748	-1,654940
	18	1	-0,754022	1,857759	-2,345522
Pr-G7	1	6	-0,582197	2,467410	-0,000604
	2	14	-0,797182	0,614641	-0,000294
	3	53	1,583950	-0,295325	0,000119
	4	7	-1,805160	-0,066635	1,235111
	5	6	-2,710748	-0,990246	0,670212
	6	6	-2,710645	-0,990859	-0,669673
	7	7	-1,804839	-0,067879	-1,235335
	8	1	-1,620241	-0,125637	-2,220512
	9	1	-1,621689	-0,122374	2,220602
	10	1	-3,327206	-1,603593	1,304880
	11	1	-3,326953	-1,604836	-1,303879
	12	1	-0,018539	2,785243	-0,878005
	13	1	-1,556653	2,956376	-0,004733
	14	1	-0,026017	2,785830	0,881395

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-A8	1	14	1,757176	-0,000001	-0,000001
	2	15	0,114095	-1,568426	0,000000
	3	15	-1,109985	0,000001	1,095260
	4	15	-1,109987	0,000000	-1,095259
	5	15	0,114097	1,568426	-0,000001
	6	1	2,638119	-0,000001	-1,201241
	7	1	2,638120	-0,000002	1,201239
Pr-B8	1	7	2,314408	-1,056374	0,846743
	2	14	1,254028	0,000199	-0,000383
	3	15	-0,397088	1,179659	1,043998
	4	15	-1,608865	-0,721533	0,818382
	5	15	-1,610788	0,721018	-0,817506
	6	15	-0,397315	-1,178774	-1,044956
	7	7	2,316642	1,055465	-0,846186
	8	1	1,970193	1,876309	-1,314975
	9	1	3,151994	0,700020	-1,285003
	10	1	1,966161	-1,876877	1,314789
	11	1	3,148759	-0,701412	1,287884
Pr-C8	1	6	-1,275446	-1,431240	0,027593
	2	6	-2,626096	-0,696048	0,325113
	3	6	-2,625741	0,696640	-0,326177
	4	6	-1,275113	1,431518	-0,027846
	5	14	-0,932889	2,723338	-1,369846
	6	14	-0,934010	-2,722747	1,370098
	7	14	-1,350281	-2,303602	-1,657937
	8	14	-0,000284	0,000002	-0,000024
	9	15	1,669544	-0,068692	-1,567787
	10	15	2,886771	1,091591	-0,047536
	11	15	2,886552	-1,092163	0,047836
	12	15	1,669360	0,068356	1,567936
	13	14	-1,350483	2,303425	1,657902
	14	1	-1,577152	-1,334348	-2,761925
	15	1	-0,090584	-3,036019	-1,933086
	16	1	-2,481611	-3,267980	-1,656566
	17	1	-2,057077	3,694632	-1,430679
	18	1	-2,058467	-3,693730	1,430838
	19	1	-2,481985	3,267601	1,656517
	20	1	-1,577405	1,333874	2,761618
	21	1	-0,090966	3,035988	1,933490
	22	1	0,319633	-3,469774	1,103304
	23	1	-0,830924	-2,055916	2,694038
	24	1	0,320848	3,469980	-1,102428
	25	1	-0,829544	2,056861	-2,693945
	26	1	-3,484358	1,277329	0,020750
	27	1	-2,756277	0,579629	-1,405867
	28	1	-3,484634	-1,276542	-0,022339
	29	1	-2,757277	-0,579018	1,404723

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Pr-D8	1	6	3,235052	-0,650670	-0,408300
	2	6	3,235098	0,650629	0,408243
	3	7	1,889810	0,766753	0,982225
	4	14	0,693834	0,000027	0,000046
	5	15	-0,950112	-1,174956	1,051258
	6	15	-2,162688	-0,725206	-0,813039
	7	15	-2,162807	0,725161	0,812969
	8	15	-0,950094	1,174997	-1,051211
	9	7	1,889727	-0,766748	-0,982200
	10	1	1,727930	-1,558152	-1,581055
	11	1	1,728080	1,558152	1,581105
	12	1	3,995675	0,607814	1,190218
	13	1	3,995585	-0,607878	-1,190318
	14	1	3,473476	1,497480	-0,246255
	15	1	3,473443	-1,497528	0,246185
Pr-E8	1	6	-1,766939	1,458168	0,000400
	2	14	-0,544256	0,090017	-0,000420
	3	15	1,115718	0,011297	-1,572569
	4	15	2,309482	-1,107672	-0,000759
	5	15	2,355606	1,071449	0,001405
	6	15	1,114965	0,008168	1,572605
	7	6	-3,103782	1,211573	0,000841
	8	6	-3,717660	-0,083768	0,000630
	9	6	-3,005924	-1,236874	-0,000606
	10	7	-1,636329	-1,296808	-0,001605
	11	1	-1,259095	-2,231815	-0,002581
	12	1	-3,516652	-2,191821	-0,000894
	13	1	-4,795081	-0,151523	0,001259
	14	1	-3,785199	2,057897	0,001238
	15	1	-1,440813	2,491458	0,000284
Pr-F8	1	1	2,958165	2,747523	0,000046
	2	6	2,544837	1,747254	-0,000010
	3	6	3,369477	0,687801	0,000085
	4	6	2,952626	-0,706536	0,000016
	5	6	3,841758	-1,716121	0,000115
	6	7	1,154852	1,684676	-0,000190
	7	14	0,269127	0,191999	-0,000102
	8	7	1,563081	-0,948641	-0,000189
	9	15	-1,347573	-0,044135	-1,578798
	10	15	-2,390762	-1,297695	0,000146
	11	15	-1,347414	-0,043931	1,578811
	12	15	-2,706478	0,858250	0,000021
	13	1	4,900778	-1,511980	0,000239
	14	1	3,530351	-2,751641	0,000065
	15	1	4,432583	0,873032	0,000219
	16	1	1,333682	-1,931059	-0,000282
	17	1	0,682346	2,572177	-0,000124

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
TS-A1	1	14	-0,132445	0,000000	-0,119208
	2	1	-0,400024	1,214667	0,694293
	3	1	-0,400021	-1,214666	0,694294
	4	1	1,360076	0,000000	-0,430536
	5	1	1,294197	0,000002	0,710857
Ts-B1	1	7	1,497319	-0,398727	0,060841
	2	14	0,000015	0,428753	-0,201128
	3	7	-1,497387	-0,398683	0,060835
	4	1	2,072951	-0,605009	-0,737743
	5	1	1,656078	-1,056843	0,805694
	6	1	-1,655782	-1,056927	0,805661
	7	1	-2,072749	-0,605350	-0,737851
	8	1	0,000050	1,787109	0,470899
	9	1	-0,000279	1,116349	1,357406
Ts-C1	1	6	1,453135	0,025663	0,094796
	2	14	-0,011344	-0,051966	-1,155597
	3	6	-1,448756	-0,018422	0,118401
	4	14	-2,271044	1,691862	0,076283
	5	6	0,707119	0,353150	1,435797
	6	6	-0,696520	-0,284297	1,461296
	7	14	2,635024	1,427798	-0,371590
	8	14	2,392082	-1,612186	0,183550
	9	14	-2,752098	-1,335207	-0,255627
	10	1	1,590481	-2,630085	0,909168
	11	1	2,692318	-2,113467	-1,181798
	12	1	3,685901	-1,444488	0,904710
	13	1	-4,040561	-1,039856	0,428688
	14	1	3,588659	1,694536	0,738383
	15	1	-3,126619	1,868185	1,279795
	16	1	-1,266127	2,787695	0,060272
	17	1	-3,112168	1,818847	-1,140508
	18	1	3,412074	1,079195	-1,588182
	19	1	1,865796	2,673447	-0,631556
	20	1	-3,023816	-1,405119	-1,714649
	21	1	-2,258715	-2,655001	0,213902
	22	1	-1,256138	0,095610	2,320435
	23	1	-0,587820	-1,361516	1,606981
	24	1	1,283132	0,019205	2,302578
	25	1	0,600426	1,436375	1,546831
	26	1	-0,015304	-1,200062	-2,171071
	27	1	-0,018066	-1,764292	-1,223993

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-D1	1	6	-1,180951	0,818383	0,250102
	2	7	0,091293	1,228524	-0,365088
	3	14	1,216431	-0,067931	-0,106392
	4	7	0,002761	-1,294627	0,032358
	5	6	-1,338613	-0,687448	-0,037115
	6	1	0,333975	2,196716	-0,229669
	7	1	0,093237	-2,167459	-0,458082
	8	1	-2,016557	-1,133396	0,695442
	9	1	-2,019467	1,370517	-0,178285
	10	1	-1,774813	-0,824149	-1,031493
	11	1	-1,176229	0,982889	1,335513
	12	1	2,428305	0,001630	0,765124
	13	1	1,560524	0,201397	1,642125
Ts-E1	1	6	0,256430	1,480547	-0,143965
	2	6	-1,070647	1,240479	-0,037972
	3	6	-1,681586	-0,049171	0,173774
	4	6	-1,023176	-1,225400	0,040220
	5	7	0,320499	-1,325985	-0,240741
	6	14	1,407402	0,040795	-0,051129
	7	1	0,648267	-2,241030	-0,498323
	8	1	-1,563630	-2,162078	0,114010
	9	1	-2,741531	-0,087863	0,377494
	10	1	-1,756078	2,078134	-0,135562
	11	1	0,601904	2,485145	-0,347566
	12	1	2,472991	-0,115436	1,003700
	13	1	1,504835	0,075160	1,694899
Ts-F1	1	6	2,626327	-0,294809	0,056063
	2	6	1,302676	-0,065356	-0,009979
	3	7	0,383638	-1,095634	-0,298429
	4	14	-1,306463	-0,954296	0,008769
	5	7	-1,602709	0,742985	-0,194314
	6	6	-0,548639	1,628261	-0,013530
	7	6	0,743089	1,276005	0,135990
	8	1	-1,243217	-0,899040	1,744600
	9	1	-1,979202	-1,671933	1,133323
	10	1	0,800234	-1,968995	-0,574105
	11	1	1,454204	2,065152	0,329060
	12	1	-0,823381	2,675836	0,015949
	13	1	-2,480327	1,132342	-0,486700
	14	1	3,317215	0,518744	0,212629
	15	1	3,037729	-1,288038	-0,059577

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-A2	1	8	-1.217171	-0.102585	-0.101178
	2	14	0.699210	-0.007961	0.099626
	3	1	1.032371	1.325096	-0.496635
	4	1	1.176914	-0.978113	-0.931882
	5	1	-1.631146	0.768232	-0.179717
	6	1	-0.629719	-0.183072	1.022886
Ts-B2	1	8	1.636536	-0.568357	0.327924
	2	14	-0.067109	-0.018955	-0.478680
	3	7	-0.337182	1.545139	0.217354
	4	7	-1.308869	-1.005461	0.188258
	5	1	2.125032	0.193913	0.675278
	6	1	1.435185	-0.431876	-0.939251
	7	1	0.019737	2.365137	-0.245315
	8	1	-1.202428	1.752248	0.692914
	9	1	-1.365889	-1.974921	-0.077504
	10	1	-1.642042	-0.870024	1.132725
Ts-C2	1	6	1.421867	0.148286	0.214630
	2	14	2.782731	-1.171841	0.202016
	3	14	2.215426	1.811342	-0.254271
	4	14	0.018597	-0.201167	-1.029527
	5	6	-1.417726	0.202520	0.187337
	6	14	-2.611854	1.428012	-0.626639
	7	6	0.697085	0.224146	1.596379
	8	6	-0.695507	0.849104	1.420886
	9	8	0.065377	-2.141755	-1.329716
	10	14	-2.387702	-1.329061	0.718989
	11	1	-0.799652	-2.578827	-1.304472
	12	1	0.029776	-1.281747	-2.260047
	13	1	2.284507	-2.422619	0.825411
	14	1	3.946169	-0.697121	1.001112
	15	1	3.255703	-1.448805	-1.175724
	16	1	3.115659	1.648688	-1.422297
	17	1	2.999167	2.321271	0.901422
	18	1	1.196655	2.838742	-0.600495
	19	1	-3.572517	1.954008	0.379647
	20	1	-3.381661	0.768700	-1.712548
	21	1	-1.862869	2.578674	-1.194138
	22	1	-0.585330	1.926648	1.265996
	23	1	0.583502	-0.783851	2.004323
	24	1	-1.279552	0.739776	2.339021
	25	1	1.274858	0.789968	2.332126
	26	1	-2.730563	-2.186855	-0.451089
	27	1	-3.663829	-0.940698	1.373627
	28	1	-1.608132	-2.158266	1.672500

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-D2	1	6	1.511589	-0.766929	0.469535
	2	7	0.398184	-1.227079	-0.369224
	3	14	-0.772726	0.016178	-0.622668
	4	8	-2.169180	-0.104973	0.734186
	5	6	1.674858	0.727220	0.160793
	6	7	0.318178	1.250130	-0.059563
	7	1	-2.389709	0.124351	-0.525242
	8	1	-2.238593	0.699546	1.272392
	9	1	0.183621	-2.208919	-0.325099
	10	1	0.280260	2.196315	-0.401545
	11	1	1.299464	-0.902336	1.537236
	12	1	2.166982	1.234720	0.993722
	13	1	2.303847	0.852891	-0.728054
	14	1	2.432525	-1.306370	0.240004
Ts-E2	1	6	0.178102	1.452752	-0.266248
	2	14	-1.001327	0.083890	-0.607520
	3	8	-2.302934	0.072956	0.885673
	4	6	1.446639	1.216192	0.162549
	5	6	2.027910	-0.074684	0.375994
	6	6	1.370224	-1.232467	0.119232
	7	7	0.079750	-1.290659	-0.337685
	8	1	-0.126169	2.482955	-0.407382
	9	1	-0.239798	-2.219848	-0.562389
	10	1	1.868760	-2.184481	0.256489
	11	1	3.045856	-0.137036	0.731126
	12	1	2.095740	2.065223	0.360843
	13	1	-2.587607	-0.158259	-0.353844
	14	1	-2.310229	-0.742802	1.409693
Ts-F2	1	6	2.652062	-1.111670	0.137741
	2	6	1.522467	-0.390291	0.013125
	3	6	1.474942	1.033011	0.311405
	4	6	0.396663	1.822956	0.173456
	5	7	-0.856525	1.404152	-0.254105
	6	14	-1.250295	-0.257335	-0.577097
	7	8	-2.302857	-0.825624	0.944937
	8	7	0.318184	-0.972391	-0.436681
	9	1	-1.958555	-1.590551	1.432860
	10	1	2.682161	-2.168408	-0.090016
	11	1	3.567423	-0.643850	0.464613
	12	1	2.392926	1.485171	0.654922
	13	1	0.477038	2.878387	0.401455
	14	1	-1.558218	2.121753	-0.308896
	15	1	0.429711	-1.930662	-0.730859
	16	1	-2.613924	-1.090518	-0.283089

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-G2	1	6	1.658206	-0.639613	0.324507
	2	6	1.631843	0.702147	0.296069
	3	7	0.419547	1.218156	-0.194263
	4	14	-0.716057	-0.041989	-0.607289
	5	8	-2.134820	-0.077727	0.729143
	6	7	0.476352	-1.226261	-0.152591
	7	1	2.429724	1.360230	0.596399
	8	1	2.479748	-1.251026	0.658309
	9	1	0.408901	-2.226242	-0.198990
	10	1	0.355691	2.200297	-0.390925
	11	1	-2.334631	0.082965	-0.555871
	12	1	-2.247660	0.724960	1.264518
Ts-A3	1	6	-1.661453	0.275610	0.018768
	2	8	-0.534046	-0.604086	0.100641
	3	14	1.217812	0.088557	-0.089845
	4	1	1.899810	-0.338938	1.172179
	5	1	1.004157	1.557879	0.114562
	6	1	0.139520	-0.776162	-0.957284
	7	1	-1.681742	0.907767	0.908034
	8	1	-1.601949	0.913997	-0.866354
	9	1	-2.568075	-0.325309	-0.031036
Ts-B3	1	6	-2.267058	0.022704	0.289533
	2	8	-1.141226	-0.786785	-0.040156
	3	14	0.614525	-0.022675	-0.515240
	4	7	0.640318	1.567704	0.150101
	5	7	1.791991	-0.888965	0.393431
	6	1	-0.691299	-0.656392	-1.241474
	7	1	-2.194857	0.349324	1.327370
	8	1	-2.321837	0.915436	-0.343655
	9	1	-3.181168	-0.557376	0.157683
	10	1	1.924500	-1.871832	0.219608
	11	1	2.004417	-0.659870	1.354105
	12	1	1.273270	1.847743	0.882667
	13	1	0.289610	2.357294	-0.363622

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-C3	1	6	1.371206	-0.467722	0.242268
	2	14	2.887796	0.615281	0.549569
	3	14	-0.010911	0.189762	-0.924250
	4	8	-0.271012	2.136448	-0.966693
	5	6	0.677643	3.189193	-0.741410
	6	6	-1.458509	-0.385543	0.199252
	7	14	-2.778714	-1.285633	-0.818607
	8	6	0.629634	-0.828389	1.573849
	9	6	-0.787976	-1.338357	1.248775
	10	14	2.010685	-2.033237	-0.648887
	11	14	-2.270501	1.098658	1.072501
	12	1	-0.092532	1.444056	-2.008027
	13	1	0.271627	4.114216	-1.160920
	14	1	1.640134	2.968067	-1.218850
	15	1	0.828888	3.311560	0.334835
	16	1	-1.282718	1.967622	1.770953
	17	1	-3.083630	1.928323	0.149180
	18	1	-3.179253	0.553673	2.123321
	19	1	-3.345561	-0.404133	-1.873455
	20	1	-3.899208	-1.748982	0.050805
	21	1	-2.187752	-2.490471	-1.465978
	22	1	2.694690	-2.911997	0.340906
	23	1	2.975043	-1.662521	-1.717944
	24	1	0.914597	-2.821725	-1.276824
	25	1	3.984507	-0.177431	1.175620
	26	1	3.419057	1.197476	-0.712319
	27	1	2.551895	1.725469	1.484035
	28	1	1.179520	-1.575067	2.162884
	29	1	0.550318	0.067496	2.204636
	30	1	-0.715375	-2.357999	0.843184
	31	1	-1.385109	-1.421940	2.166533
Ts-D3	1	6	-2.580082	0.614252	0.637921
	2	8	-1.861302	-0.538554	0.191962
	3	14	-0.197289	-0.477131	-0.808057
	4	7	1.063753	-1.240305	0.094671
	5	6	1.844423	-0.278268	0.880183
	6	6	1.821907	1.028917	0.076948
	7	7	0.496810	1.097860	-0.554067
	8	1	-1.774748	-0.790393	-1.071401
	9	1	1.015661	-2.177732	0.456269
	10	1	0.374393	1.854889	-1.205643
	11	1	1.405610	-0.110689	1.871871
	12	1	1.995651	1.882400	0.736634
	13	1	2.623311	1.014229	-0.671000
	14	1	2.871536	-0.619808	1.023342
	15	1	-3.624058	0.346335	0.800960
	16	1	-2.148624	0.969397	1.573873
	17	1	-2.527690	1.427346	-0.092338

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-E3	1	14	0.446888	-0.542165	-0.883248
	2	7	-0.303416	1.060529	-0.793802
	3	6	-1.429155	1.397938	-0.090506
	4	6	-2.182807	0.506174	0.599692
	5	6	-1.893385	-0.895633	0.633340
	6	6	-0.827022	-1.498181	0.042558
	7	8	2.050230	-0.500007	0.235925
	8	1	2.076818	-0.572112	-1.040627
	9	6	2.555996	0.638317	0.935053
	10	1	2.455798	1.553444	0.343263
	11	1	2.000020	0.765698	1.864927
	12	1	3.609608	0.480532	1.165123
	13	1	0.098156	1.818986	-1.321959
	14	1	-1.714748	2.442620	-0.123153
	15	1	-3.055625	0.872785	1.119393
	16	1	-2.604090	-1.511964	1.178244
	17	1	-0.742058	-2.575010	0.128667
Ts-F3	1	6	2.431685	-1.759248	-0.016606
	2	6	1.606248	-0.696016	-0.052769
	3	7	0.398141	-0.719596	-0.779865
	4	14	-0.845465	0.482549	-0.883171
	5	8	-2.297344	-0.039308	0.235769
	6	6	-2.449200	-1.270687	0.958328
	7	6	1.917371	0.548380	0.634133
	8	6	1.161012	1.659156	0.612062
	9	7	-0.054321	1.789358	-0.045450
	10	1	2.197926	-2.680430	-0.532644
	11	1	3.361245	-1.713235	0.528849
	12	1	2.843346	0.576656	1.188147
	13	1	1.499114	2.543715	1.137471
	14	1	-0.493270	2.690447	0.030503
	15	1	0.285259	-1.560032	-1.325680
	16	1	-2.424698	0.070095	-1.034163
	17	1	-3.500814	-1.409241	1.204499
	18	1	-2.097575	-2.122031	0.371377
	19	1	-1.864708	-1.215021	1.876190

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-G3	1	6	-2.492677	0.639694	0.683617
	2	8	-1.815924	-0.499831	0.136799
	3	14	-0.122552	-0.552115	-0.778733
	4	7	1.079906	-1.145417	0.338306
	5	6	1.968614	-0.143654	0.756522
	6	6	1.728609	1.047147	0.184770
	7	7	0.636117	1.020990	-0.698526
	8	1	2.290608	1.952492	0.341841
	9	1	2.755788	-0.363542	1.458252
	10	1	1.198857	-2.080491	0.682219
	11	1	0.465364	1.820714	-1.280242
	12	1	-1.708965	-0.782382	-1.123899
	13	1	-3.565413	0.450492	0.698439
	14	1	-2.142173	0.801191	1.703295
	15	1	-2.290378	1.541656	0.100049
Ts-A4	1	7	1.192131	0.013791	-0.051305
	2	14	-0.713640	-0.027700	0.083634
	3	1	1.729165	0.728666	-0.531226
	4	1	1.681101	-0.870355	-0.032707
	5	1	0.513722	0.024393	1.143037
	6	1	-1.023425	1.347255	-0.410098
	7	1	-1.254522	-0.938701	-0.980748
Ts-B4	1	7	1.116786	-1.223151	0.222107
	2	14	-0.111041	0.079019	-0.472460
	3	7	0.650905	1.497354	0.192852
	4	7	-1.624047	-0.329572	0.275683
	5	1	0.833383	-1.047831	-1.134999
	6	1	0.489275	2.389123	-0.249161
	7	1	0.713446	1.607114	1.197795
	8	1	-2.404463	-0.621414	-0.288525
	9	1	-1.924953	0.060554	1.157308
	10	1	0.787909	-2.113956	0.570874
	11	1	2.054470	-0.992268	0.526661

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-C4	1	6	1.416882	0.154518	0.213727
	2	14	2.109011	1.855988	-0.276004
	3	14	2.846006	-1.073101	0.230801
	4	6	0.689833	0.206593	1.594712
	5	6	-0.706909	0.825234	1.423506
	6	6	-1.431043	0.188451	0.187915
	7	14	-2.394326	-1.351611	0.707617
	8	14	0.005721	-0.259119	-1.030781
	9	7	0.102947	-2.155737	-1.330949
	10	14	-2.614664	1.420050	-0.624811
	11	1	0.581506	-0.805894	1.994640
	12	1	-1.289142	0.703984	2.341582
	13	1	-3.620680	1.905809	0.358855
	14	1	-1.865532	2.599947	-1.128543
	15	1	-3.339622	0.789769	-1.757897
	16	1	-2.961074	-2.068252	-0.464991
	17	1	-1.539266	-2.307445	1.459597
	18	1	-3.521604	-0.962736	1.596181
	19	1	3.014433	1.732650	-1.444918
	20	1	1.030867	2.817243	-0.626446
	21	1	2.873496	2.427009	0.866497
	22	1	3.444957	-1.239737	-1.117205
	23	1	3.915618	-0.644366	1.171088
	24	1	2.366093	-2.407360	0.691998
	25	1	0.432371	-1.233705	-2.278381
	26	1	-0.708012	-2.592593	-1.751331
	27	1	0.665437	-2.838129	-0.825926
	28	1	1.263029	0.769577	2.336585
	29	1	-0.600572	1.904713	1.280593
Ts-D4	1	6	-1.753070	-0.609622	0.210088
	2	6	-1.458864	0.883440	0.408451
	3	7	-0.310137	1.176262	-0.451258
	4	14	0.760113	-0.184973	-0.599292
	5	7	-0.447374	-1.266940	0.055466
	6	7	2.199268	0.092884	0.661597
	7	1	2.371823	0.096206	-0.716832
	8	1	2.699675	-0.731829	0.980457
	9	1	2.281582	0.848716	1.343075
	10	1	-0.493332	-2.234910	-0.217561
	11	1	-1.248358	1.076934	1.469221
	12	1	-2.297254	-1.006150	1.071321
	13	1	-2.384768	-0.743595	-0.676354
	14	1	-0.063185	2.143753	-0.564141
	15	1	-2.328465	1.482146	0.129038

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-E4	1	6	-0.063663	1.405981	-0.346318
	2	14	1.002303	-0.084464	-0.597868
	3	7	2.270541	0.053029	0.841784
	4	6	-1.346240	1.300210	0.084733
	5	6	-2.024342	0.072699	0.396366
	6	6	-1.473762	-1.148843	0.194458
	7	7	-0.206709	-1.350392	-0.291934
	8	1	0.307461	2.397074	-0.583372
	9	1	0.022060	-2.313335	-0.478187
	10	1	-2.048577	-2.043696	0.403451
	11	1	-3.035728	0.116663	0.772844
	12	1	-1.935606	2.206306	0.201708
	13	1	2.618163	0.175978	-0.479439
	14	1	2.241290	0.719422	1.615200
	15	1	2.799906	-0.774667	1.093577
Ts-F4	1	6	-2.622522	-1.125786	0.130937
	2	6	-1.497800	-0.395057	-0.000418
	3	6	-1.456775	1.016565	0.356507
	4	6	-0.398893	1.832135	0.203308
	5	7	0.849525	1.448443	-0.267729
	6	14	1.269762	-0.222016	-0.577344
	7	7	2.156728	-0.976157	0.942036
	8	7	-0.311565	-0.942395	-0.521337
	9	1	1.510308	2.192818	-0.404663
	10	1	-0.494047	2.879622	0.462984
	11	1	-2.368255	1.440469	0.750111
	12	1	-3.530745	-0.673061	0.496927
	13	1	-2.656502	-2.172644	-0.138476
	14	1	-0.427502	-1.878336	-0.876625
	15	1	2.993441	-0.521424	1.293255
	16	1	1.712457	-1.539529	1.666344
	17	1	2.477298	-1.296079	-0.379839
Ts-G4	1	6	-1.608855	0.750061	0.278525
	2	6	-1.694938	-0.587141	0.341541
	3	7	-0.533182	-1.244233	-0.104977
	4	14	0.711487	-0.111976	-0.603032
	5	7	-0.374411	1.213448	-0.209852
	6	7	2.122769	0.053440	0.683071
	7	1	-2.541516	-1.149868	0.699198
	8	1	-2.379843	1.445050	0.568057
	9	1	-0.313284	2.165347	-0.522196
	10	1	2.303082	0.293803	-0.682874
	11	1	-0.564225	-2.236481	-0.250656
	12	1	2.708612	-0.762703	0.838703
	13	1	2.142889	0.676411	1.494119

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-A5	1	7	-0.542527	-0.515360	0.000387
	2	7	-1.733173	0.298747	0.132215
	3	14	1.236758	0.051287	-0.034088
	4	1	1.672162	0.523751	1.328054
	5	1	1.038411	1.320720	-0.800775
	6	1	0.357724	-1.028771	-0.908942
	7	1	-2.359821	0.069963	-0.632858
	8	1	-0.652807	-1.346860	0.571363
	9	1	-1.440382	1.259467	-0.007829
Ts-B5	1	7	-0.448916	-0.093691	0.077054
	2	14	0.153559	-0.052055	1.701595
	3	7	2.040053	-0.069251	1.907454
	4	7	2.946610	1.049548	1.771317
	5	7	-0.060275	1.654205	2.115861
	6	1	-0.321071	0.670355	-0.572295
	7	1	-0.579331	-0.969878	-0.399564
	8	1	-0.079605	1.884084	3.099167
	9	1	-0.854629	2.095262	1.673806
	10	1	1.204204	-0.651651	2.842392
	11	1	3.532016	1.088265	2.599986
	12	1	2.468142	-0.908999	1.524112
	13	1	2.344328	1.869201	1.789759

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-C5	1	6	-1.501577	-0.286264	0.198285
	2	14	-0.023708	0.149770	-0.980427
	3	7	0.184381	2.036603	-1.193850
	4	7	0.868649	2.943509	-0.317624
	5	6	-0.835576	-1.053064	1.392072
	6	6	0.603921	-0.556633	1.602781
	7	6	1.336485	-0.451947	0.228156
	8	14	1.860950	-2.169099	-0.407173
	9	14	-2.757059	-1.381046	-0.701243
	10	14	-2.374884	1.273351	0.796515
	11	14	2.944148	0.552472	0.350865
	12	1	-1.464167	2.136370	1.601639
	13	1	-2.873223	2.096910	-0.336941
	14	1	-3.535772	0.934294	1.661019
	15	1	4.062283	-0.374917	0.694517
	16	1	-3.800182	-1.860934	0.246542
	17	1	2.524188	-2.923960	0.689969
	18	1	0.704029	-2.977332	-0.877866
	19	1	2.807473	-2.029176	-1.541689
	20	1	-3.433645	-0.630148	-1.790230
	21	1	-2.086177	-2.572545	-1.279939
	22	1	3.308207	1.198757	-0.933372
	23	1	2.868258	1.552379	1.442570
	24	1	1.128306	-1.217048	2.299464
	25	1	0.577288	0.428369	2.076209
	26	1	-1.411568	-0.947949	2.316055
	27	1	-0.813857	-2.125970	1.178988
	28	1	0.578264	1.158958	-2.142097
	29	1	-0.601998	2.445041	-1.701107
	30	1	1.122694	3.783211	-0.824893
	31	1	0.256608	3.196073	0.454195
Ts-D5	1	6	1.814799	-0.070259	0.921964
	2	7	1.050986	-1.195179	0.382038
	3	14	-0.219807	-0.710532	-0.702463
	4	7	-1.925450	-0.331578	0.003997
	5	7	-2.433425	0.819048	0.742589
	6	6	1.759718	1.015528	-0.159221
	7	7	0.420759	0.939886	-0.758975
	8	1	-1.760384	-0.600362	-1.348510
	9	1	1.103674	-2.066641	0.879938
	10	1	0.347921	1.458656	-1.620356
	11	1	1.947553	1.998849	0.280094
	12	1	2.850408	-0.347458	1.131387
	13	1	2.546930	0.824825	-0.898955
	14	1	1.379551	0.313824	1.854759
	15	1	-1.781750	1.560294	0.493080
	16	1	-2.536472	-1.126957	0.169456
	17	1	-2.257327	0.635570	1.729596

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-E5	1	6	-0.784019	1.516794	0.098194
	2	14	0.471384	0.590237	-0.904133
	3	7	2.085265	0.239462	0.088926
	4	7	2.297805	-0.746638	1.109302
	5	6	-1.823523	0.886190	0.707323
	6	6	-2.119243	-0.511957	0.616213
	7	6	-1.410636	-1.362857	-0.171185
	8	7	-0.326952	-0.998083	-0.914154
	9	1	0.053636	-1.735267	-1.485428
	10	1	-1.715265	-2.399615	-0.255575
	11	1	-2.969321	-0.904698	1.154034
	12	1	-2.513186	1.477428	1.305835
	13	1	-0.705322	2.591784	0.215131
	14	1	2.040106	0.232288	-1.283619
	15	1	1.760859	-0.493946	1.934148
	16	1	2.601525	1.113770	0.222424
	17	1	3.279286	-0.777270	1.359131
Ts-F5	1	6	-2.410644	-1.726247	-0.060442
	2	6	-1.580346	-0.664976	-0.092335
	3	7	-0.413635	-0.654222	-0.873695
	4	14	0.875381	0.511486	-0.898495
	5	7	2.269153	-0.299894	0.112338
	6	7	2.188634	-1.351186	1.080714
	7	6	-1.868994	0.549580	0.658825
	8	6	-1.109069	1.657902	0.668256
	9	7	0.104134	1.801456	0.007439
	10	1	2.280180	-0.253515	-1.283541
	11	1	-0.300608	-1.491613	-1.423569
	12	1	-2.783876	0.557216	1.231811
	13	1	-1.436596	2.524393	1.230328
	14	1	0.503219	2.723490	0.032814
	15	1	-3.316887	-1.695388	0.524046
	16	1	-2.202990	-2.628982	-0.618348
	17	1	1.640228	-1.038145	1.875293
	18	1	3.021916	0.374284	0.277918
	19	1	3.116387	-1.603184	1.398776

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-G5	1	6	-1.932392	-0.001163	-0.758962
	2	6	-1.663412	1.062799	0.012370
	3	7	-0.550543	0.880015	0.856470
	4	14	0.152881	-0.735957	0.684162
	5	7	1.851386	-0.325723	-0.024862
	6	7	2.251096	0.769666	-0.875286
	7	7	-1.062926	-1.082835	-0.541182
	8	1	-1.273874	-1.966403	-0.967755
	9	1	-0.483011	1.467742	1.668471
	10	1	-2.208315	1.992640	0.016266
	11	1	-2.719662	-0.065695	-1.492460
	12	1	1.690707	-0.647601	1.340072
	13	1	1.531951	1.476800	-0.756341
	14	1	2.355675	-1.169628	-0.296376
	15	1	3.117940	1.157862	-0.516582
Ts-A6	1	6	1,136126	1,344432	-0,008192
	2	17	0,709694	-0,911042	0,003410
	3	14	-1,338842	0,269133	-0,016463
	4	1	0,750265	1,818778	0,878194
	5	1	0,824368	1,775999	-0,943487
	6	1	2,158415	1,009162	0,044721
	7	1	-1,849466	-0,331896	1,269066
	8	1	-2,021347	-0,618779	-1,026839
Ts-B6	1	6	1,827490	-0,418178	1,261665
	2	17	1,344522	0,316628	-0,952247
	3	14	-0,738328	-0,166205	0,505221
	4	7	-1,612632	1,311679	0,343275
	5	7	-1,608642	-1,261600	-0,503851
	6	1	-1,266081	2,148721	0,782814
	7	1	-2,159285	1,534736	-0,477343
	8	1	-1,260996	-2,196613	-0,641283
	9	1	-2,145793	-0,955715	-1,303860
	10	1	2,803466	-0,278154	0,831725
	11	1	1,547797	0,288224	2,023627

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-C6	1	6	-0,297854	2,699224	2,056264
	2	17	-0,137744	2,517746	-0,249943
	3	14	-0,027667	0,291875	0,750819
	4	6	-1,379355	-0,632185	-0,279579
	5	14	-1,990933	-2,074698	0,799636
	6	6	-0,615316	-1,128603	-1,542645
	7	6	0,790764	-1,598551	-1,143616
	8	6	1,455556	-0,544509	-0,192833
	9	14	2,545554	0,637532	-1,193420
	10	14	2,555655	-1,388044	1,099255
	11	14	-2,904960	0,400317	-0,711260
	12	1	1,813938	1,203982	-2,354131
	13	1	3,079125	1,741571	-0,359780
	14	1	3,700522	-0,133493	-1,732133
	15	1	-4,045588	-0,489830	-1,067245
	16	1	3,559042	-2,260470	0,432228
	17	1	-2,629833	-3,100240	-0,066451
	18	1	-0,893715	-2,734361	1,555132
	19	1	-2,987795	-1,587186	1,786975
	20	1	3,280067	-0,384141	1,921471
	21	1	1,745877	-2,243265	2,005870
	22	1	-3,335306	1,230888	0,442832
	23	1	-2,634731	1,273862	-1,879079
	24	1	-1,150766	-1,931876	-2,057816
	25	1	-0,526190	-0,307557	-2,259009
	26	1	1,396073	-1,776658	-2,037505
	27	1	0,713701	-2,568870	-0,642479
	28	1	-0,377195	3,744067	1,807758
	29	1	-1,195480	2,224916	2,413375
	30	1	0,620027	2,386969	2,523055
Ts-D6	1	6	2,725651	-0,938303	0,368635
	2	17	1,706835	1,071444	-0,446156
	3	14	0,046615	-0,758779	0,230180
	4	7	-1,119478	-0,704212	-1,047481
	5	6	-2,405176	-0,116401	-0,658616
	6	6	-2,107918	0,773246	0,555839
	7	7	-1,030198	0,098037	1,292961
	8	1	-1,108776	-1,270400	-1,877609
	9	1	-0,709527	0,578322	2,118033
	10	1	-2,999515	0,886103	1,175803
	11	1	-3,133871	-0,889726	-0,387889
	12	1	-1,800676	1,770201	0,218644
	13	1	-2,833151	0,478317	-1,468905
	14	1	3,566957	-0,293676	0,185861
	15	1	2,521114	-1,160655	1,401474
	16	1	2,601035	-1,758159	-0,316791

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-E6	1	6	-0,816471	1,447191	-0,308480
	2	6	-2,065635	1,255005	0,198435
	3	6	-2,686259	-0,012790	0,412307
	4	6	-2,096038	-1,187929	0,073752
	5	7	-0,859492	-1,277465	-0,501214
	6	14	0,275951	0,048653	-0,822724
	7	1	-0,569834	-2,220396	-0,710166
	8	1	-2,612646	-2,125463	0,241771
	9	1	-3,672606	-0,047009	0,850773
	10	1	-2,655497	2,125555	0,474902
	11	1	-0,468516	2,468313	-0,416818
	12	17	1,808773	-0,115351	1,199977
	13	6	2,981640	0,105798	-0,852307
	14	1	3,785342	0,120724	-0,137120
	15	1	2,901996	-0,779235	-1,458290
	16	1	2,792334	1,035939	-1,360257
Ts-F6	1	6	-3,198016	-0,483733	-0,801065
	2	17	-1,964547	-0,247951	1,234774
	3	14	-0,585531	0,161687	-0,810572
	4	7	0,765137	-0,904354	-0,601472
	5	6	2,026050	-0,662473	-0,016497
	6	6	2,307325	0,717536	0,345990
	7	6	1,464763	1,750272	0,180302
	8	7	0,186395	1,662306	-0,355286
	9	6	2,918775	-1,651639	0,174128
	10	1	-0,327881	2,526032	-0,377281
	11	1	1,775622	2,745536	0,473128
	12	1	3,276603	0,917351	0,777091
	13	1	0,631571	-1,873047	-0,850052
	14	1	2,702872	-2,675719	-0,097759
	15	1	3,883837	-1,441831	0,608388
	16	1	-3,939922	-0,700903	-0,053040
	17	1	-3,313812	0,446895	-1,328282
	18	1	-2,868271	-1,318201	-1,395195
Ts-A7	1	6	-0,934556	1,914674	-0,010168
	2	53	0,756464	-0,126883	0,000735
	3	14	-1,982120	-0,582923	-0,019338
	4	1	-1,555706	1,970114	0,868237
	5	1	-1,450168	2,007505	-0,950540
	6	1	-0,002707	2,447598	0,059293
	7	1	-1,890580	-1,298212	1,305101
	8	1	-1,836422	-1,729323	-0,989292

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-B7	1	6	0,001073	2,270946	-0,025722
	2	53	1,234946	-0,265892	0,003696
	3	14	-1,859923	0,373242	-0,010558
	4	7	-2,226646	-0,581571	1,371605
	5	7	-2,220714	-0,637608	-1,354003
	6	1	-2,016712	-0,312735	-2,285530
	7	1	-2,166266	-1,646000	-1,306002
	8	1	-2,032698	-0,216847	2,290391
	9	1	-2,171326	-1,590982	1,366857
	10	1	1,069238	2,379505	-0,023830
	11	1	-0,482982	2,573740	-0,938544
	12	1	-0,487386	2,588807	0,879712
Ts-C7	1	6	1,765610	-0,039623	2,530330
	2	53	2,324495	-0,134869	-0,117276
	3	14	-0,405816	0,037232	0,786613
	4	6	-1,344298	-1,343227	-0,223259
	5	14	-2,407248	-2,300481	1,024287
	6	6	-1,085907	1,489320	-0,298656
	7	14	0,100088	2,923008	-0,646960
	8	14	-2,533173	2,238431	0,691079
	9	6	-1,570340	0,784656	-1,598755
	10	6	-2,233279	-0,554760	-1,245632
	11	14	-0,285465	-2,613243	-1,146279
	12	1	0,424534	-1,991505	-2,291317
	13	1	0,690760	-3,283029	-0,255216
	14	1	-1,195467	-3,653973	-1,702143
	15	1	-0,677313	4,134883	-1,032046
	16	1	-3,373676	-3,175998	0,308953
	17	1	-3,428799	2,976027	-0,238250
	18	1	-3,348123	1,212780	1,392913
	19	1	-2,012938	3,179979	1,714642
	20	1	-1,558349	-3,150132	1,898892
	21	1	-3,185831	-1,371411	1,883313
	22	1	0,898094	3,268856	0,555490
	23	1	1,002414	2,588913	-1,774744
	24	1	-2,265007	1,409111	-2,168758
	25	1	-0,712847	0,599331	-2,251246
	26	1	-2,414491	-1,134964	-2,155346
	27	1	-3,222168	-0,359693	-0,818877
	28	1	2,839279	-0,102218	2,537047
	29	1	1,349970	0,907585	2,827415
	30	1	1,243623	-0,913922	2,878364

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-D7	1	6	-1,125174	2,334231	0,097847
	2	53	-1,545898	-0,474386	-0,078065
	3	14	1,192887	1,104313	0,347323
	4	7	1,905028	-0,157966	1,297153
	5	6	2,453782	-1,226108	0,445860
	6	6	2,954071	-0,536773	-0,832513
	7	7	2,056904	0,603731	-1,052485
	8	1	2,130461	1,088930	-1,928945
	9	1	1,498410	-0,469645	2,164633
	10	1	3,271633	-1,744666	0,948758
	11	1	3,989071	-0,201046	-0,703958
	12	1	1,681736	-1,960861	0,193634
	13	1	2,926736	-1,231908	-1,673745
	14	1	-2,119258	2,116082	-0,242775
	15	1	-1,040830	2,624933	1,131145
	16	1	-0,535359	2,911785	-0,593661
Ts-E7	1	6	1,623125	2,212417	0,040594
	2	53	1,597248	-0,591829	-0,024156
	3	14	-0,889071	1,286306	0,127127
	4	7	-1,771539	0,625990	-1,256530
	5	6	-2,677890	-0,395709	-1,240041
	6	6	-3,136548	-0,974165	-0,099023
	7	6	-2,707364	-0,575390	1,200304
	8	6	-1,754260	0,362962	1,464160
	9	1	-1,541759	0,958208	-2,180804
	10	1	-3,042759	-0,726741	-2,204718
	11	1	-3,867093	-1,764301	-0,189622
	12	1	-3,184956	-1,080228	2,036090
	13	1	-1,507904	0,560157	2,500733
	14	1	2,634930	1,859602	-0,023557
	15	1	1,270289	2,743829	-0,826010
	16	1	1,350477	2,645489	0,988145

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-F7	1	6	-1,913962	1,870187	-1,144487
	2	53	-1,744731	-0,644002	0,151517
	3	14	0,530154	1,351605	-0,243796
	4	7	1,188782	1,223258	1,363830
	5	6	2,194900	0,329317	1,715057
	6	6	2,873490	-0,445565	0,854029
	7	6	2,673266	-0,483329	-0,586365
	8	6	3,402088	-1,272897	-1,395076
	9	7	1,672595	0,374194	-1,094845
	10	1	0,734788	1,681286	2,135708
	11	1	2,424994	0,285241	2,772037
	12	1	3,636966	-1,096607	1,252222
	13	1	1,566294	0,297972	-2,095580
	14	1	3,244558	-1,295832	-2,464517
	15	1	4,169444	-1,912723	-0,988247
	16	1	-2,857880	1,365798	-1,226116
	17	1	-1,891691	2,709546	-0,471138
	18	1	-1,387215	2,006527	-2,073467
TS-A8	1	15	0,000000	0,000000	0,000000
	2	15	0,000000	0,000000	2,239290
	3	15	1,922985	0,000000	1,147465
	4	15	0,803697	1,906438	1,415491
	5	14	-0,488317	2,263291	-0,859125
	6	1	0,760967	3,075280	-1,052843
	7	1	-1,294289	3,075258	0,114879
Ts-B8	1	1	-2,975972	-2,037053	0,239289
	2	7	-2,293488	-1,480186	-0,249570
	3	1	-2,380977	-1,592671	-1,249856
	4	14	-1,750927	-0,007198	0,499945
	5	7	-2,337097	1,452085	-0,241007
	6	1	-2,220374	1,703198	-1,212566
	7	1	-2,546913	2,252161	0,331899
	8	15	0,581824	-0,092839	1,331118
	9	15	1,772967	1,152113	-0,086780
	10	15	1,908812	-1,059876	-0,192472
	11	15	0,206484	-0,001276	-1,163463
	28	1	2,825411	1,303273	1,850609
	29	1	1,274097	0,594348	2,252496

XYZ
Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-C8	1	6	1,317701	1,448852	0,244758
	2	14	0,387763	0,002869	-0,674338
	3	15	-1,934441	-0,427723	-1,449712
	4	15	-1,711651	0,180000	0,949999
	5	15	-3,124736	1,162707	-0,456127
	6	15	-3,463367	-0,950015	0,128499
	7	6	1,995877	0,719421	1,440296
	8	6	2,501692	-0,663679	0,997477
	9	6	1,389994	-1,427962	0,197517
	10	14	0,431509	-2,567170	1,358797
	11	14	0,374134	2,994640	0,790546
	12	14	2,593285	2,060858	-1,039318
	13	14	2,149810	-2,494332	-1,175214
	14	1	3,212216	0,951286	-1,806746
	15	1	1,931493	2,977617	-2,000232
	16	1	3,678340	2,796546	-0,334724
	17	1	3,097832	-3,487105	-0,598953
	18	1	1,340861	4,090455	1,073359
	19	1	1,305531	-3,691096	1,793779
	20	1	0,000368	-1,843087	2,582460
	21	1	-0,766675	-3,143619	0,699018
	22	1	-0,557377	3,466472	-0,263562
	23	1	-0,388030	2,740307	2,039130
	24	1	1,090321	-3,234944	-1,907537
	25	1	2,899336	-1,648706	-2,138024
	26	1	2,836289	-1,235543	1,867732
	27	1	3,390303	-0,526627	0,374414
	28	1	2,825411	1,303273	1,850609
	29	1	1,274097	0,594348	2,252496

XYZ

Calculated at the B3LYP/cc-pVTZ level

	Center	Atomic			
molecule	Number	Number	X	Y	Z
Ts-D8	1	6	3,054726	-0,577025	0,819932
	2	7	2,186526	-1,317849	-0,102723
	3	14	1,035457	-0,245354	-0,847007
	4	15	-1,380924	-0,632255	-1,178151
	5	15	-2,072558	1,241595	-0,195878
	6	15	-0,596566	0,276828	1,153539
	7	15	-2,587406	-0,716653	0,700036
	8	6	3,248012	0,811644	0,193295
	9	7	1,965221	1,177522	-0,427045
	10	1	1,977562	-2,266440	0,161883
	11	1	1,997017	1,980146	-1,033050
	12	1	3,536248	1,534035	0,960673
	13	1	4,018143	-1,076150	0,938336
	14	1	4,051979	0,768111	-0,549921
	15	1	2,605806	-0,472901	1,815986
Ts-E8	1	6	1,787483	1,285203	-0,805883
	2	6	2,835802	1,320894	0,054427
	3	6	3,311581	0,215255	0,840953
	4	6	2,895382	-1,063607	0,664449
	5	7	1,937994	-1,439350	-0,243683
	6	14	0,848608	-0,295952	-1,047079
	7	15	-1,566374	-0,775517	-1,046067
	8	15	-2,281988	1,171376	-0,241102
	9	15	-2,540784	-0,658326	0,971964
	10	15	-0,584277	0,472205	1,021357
	11	1	1,817361	-2,432743	-0,353639
	12	1	3,350870	-1,864544	1,235410
	13	1	4,087675	0,395769	1,569902
	14	1	3,384426	2,252698	0,163972
	15	1	1,533066	2,175049	-1,366703
Ts-F8	1	1	-2,785947	-2,341805	-1,387115
	2	6	-2,429436	-1,548086	-0,741595
	3	6	-2,993173	-0,326910	-0,823645
	4	6	-2,689992	0,815746	0,028882
	5	6	-3,320920	1,997464	-0,103870
	6	7	-1,392101	-1,893727	0,108823
	7	14	-0,539428	-0,672645	1,032613
	8	15	0,661839	0,393386	-0,999169
	9	15	2,772217	-0,407607	-0,988760
	10	15	2,266872	1,408895	0,170173
	11	15	1,938012	-0,596979	1,067285
	12	7	-1,738559	0,592194	1,046273
	13	1	-4,099011	2,125000	-0,840404
	14	1	-3,089269	2,840238	0,532662
	15	1	-3,765773	-0,180091	-1,563321
	16	1	-1,653917	1,351091	1,703319
	17	1	-1,122458	-2,861380	0,111035

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