

# Effect of substituents on the stabilities of multiply-substituted carbon-centered radicals

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†In memory of our dear friend and colleague Athel Beckwith, in recognition of his many outstanding contributions to chemistry.

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## Electronic Supplementary Information

(Tables S1–S6. A total of 86 pages)

**Table S1** Comparison of calculated radical stabilization energies for •CH<sub>2</sub>X radicals with experimental values (0 K, kJ mol<sup>-1</sup>)

Radical	RBMK <sup>a</sup>	UBMK <sup>a</sup>	RMPWB1K <sup>a</sup>	UMPWB1K <sup>a</sup>	RB2- PLYP <sup>a,b</sup>	UB2- PLYP <sup>a</sup>	ROB2- PLYP <sup>a,c</sup>	W1 <sup>d</sup>	Expt. <sup>e</sup>
•CH <sub>2</sub> NH <sub>2</sub>	54.8	54.5	54.7	55.1	52.4	52.1	50.9	49.3	45.8±8.4
•CH <sub>2</sub> OH	39.9	39.6	39.6	39.9	37.4	37.2	36.1	35.3	36.7±0.6
•CH <sub>2</sub> F	17.4	16.9	18.3	18.4	16.4	16.2	15.4	14.8	15.2±4.2
•CH <sub>2</sub> CH <sub>3</sub>	17.4	17.8	19.1	19.4	17.6	17.7	17.0	15.8	19.5±1.3
•CH <sub>2</sub> CF <sub>3</sub>	-5.7	-5.5	-4.1	-4.0	-3.9	-3.8	-3.6	-6.1	-6.8±4.5
•CH <sub>2</sub> SH	38.0	38.6	42.8	44.0	41.2	41.5	39.5	41.4	46.4±8.4
•CH <sub>2</sub> Cl	21.3	21.9	26.8	27.8	24.1	24.5	23.0	23.0	21.2±2.3
•CH <sub>2</sub> BH <sub>2</sub>	49.4	48.4	46.1	44.9	44.3	43.2	44.0	40.9	
•CH <sub>2</sub> CH=CH <sub>2</sub>	66.7	74.8	67.0	77.3	70.5	71.9	68.2	70.3	69.0±3.0
•CH <sub>2</sub> C≡CH	53.4	59.6	54.5	62.3	56.9	56.3	54.1	53.6	55.0±4.2 <sup>f</sup>
•CH <sub>2</sub> CHO	35.4	40.7	36.3	43.6	38.2	36.8	36.3	36.6	39.8 <sup>g,h</sup>
•CH <sub>2</sub> COOH	24.2	25.6	25.5	27.5	25.9	25.6	24.7	23.7	24.8±3.3 <sup>i</sup>
•CH <sub>2</sub> CN	31.1	36.6	32.9	40.4	36.3	34.5	33.8	33.1	33.0±4.2
MD(W1) <sup>j</sup>	1.1	2.8	2.3	4.8	2.0	1.8	0.7		
MAD(W1) <sup>j</sup>	2.9	3.5	2.9	4.8	2.0	1.8	1.3		
LD(W1) <sup>j</sup>	8.5	7.5	5.4	8.6	3.4	2.8	3.1		
MD(Expt.) <sup>j</sup>	-2.6	-0.6	-0.9	1.9	-1.1	-1.2	-2.5	-3.0	
MAD(Expt.) <sup>j</sup>	4.1	4.6	3.4	4.9	3.8	3.7	3.8	4.0	
LD(Expt.) <sup>j</sup>	-8.8	-8.3	7.8	8.2	-7.1	-7.4	-8.4	-9.3	

<sup>a</sup> Single-point energy calculations with 6-311+G(3df, 2p) basis set on geometries calculated at the UB3-LYP/6-31G(d) level; <sup>b</sup>Restricted-open-shell version of B2-PLYP<sup>1</sup> that includes 53% HF exchange and 27% MP2 correlation; <sup>c</sup>Restricted-open-shell version of B2-PLYP that includes 59% HF exchange and 28% MP2 correlation as recommended in ref 2; <sup>d</sup>W1' calculations for systems containing second-row elements; <sup>e</sup>Calculated using experimental bond dissociation energies at 298 K that were obtained from the *Handbook of Chemistry and Physics*<sup>3</sup> (and references therein), unless otherwise noted, and back-corrected to 0 K using theoretical (UB3LYP/6-31G(d)) temperature corrections (scaled by 0.9989);<sup>4</sup> <sup>f</sup>Calculated using the experimental BDE for propyne reported by Tsang;<sup>5</sup> <sup>g</sup>Species without experimental error bars are not included in the statistics; <sup>h</sup>Calculated using the experimental BDE for acetaldehyde reported by Cummings and Kebarle;<sup>6</sup> <sup>i</sup>Calculated using the experimental BDE for acetic acid reported by Lagoa et al.;<sup>7</sup> <sup>j</sup>MD, MAD and LD are mean deviation, mean absolute deviation and the largest deviation respectively from W1 and from experimental values.

**Table S2** ROB2-PLYP and UB2-PLYP- total energies<sup>a</sup> of substituted methanes (CHXYZ) and substituted radicals ( $\bullet$ CXYZ) (0 K, Hartrees)

	#	X	Y	Z	ROB2-PLYP <sup>b</sup>		UB2-PLYP <sup>b</sup>	
					CHXYZ	$\bullet$ CXYZ	CHXYZ	$\bullet$ CXYZ
	1	H	H	H	-40.44399	-39.78275	-40.44556	-39.78564
{ $\pi_d$ }	2	F	H	H	-139.66747	-139.01211	-139.67463	-139.02088
	3	Cl	H	H	-499.95596	-499.30349	-499.96290	-499.31231
	4	NH <sub>2</sub>	H	H	-95.74969	-95.10784	-95.75473	-95.11466
	5	OH	H	H	-115.63194	-114.98447	-115.63858	-114.99283
	6	SH	H	H	-438.55893	-437.91275	-438.56527	-437.92115
	7	F	F	H	-238.91112	-238.25560	-238.92379	-238.26978
	8	Cl	F	H	-599.18727	-598.53543	-599.20000	-598.54986
	9	NH <sub>2</sub>	F	H	-194.99754	-194.34528	-195.00821	-194.35757
	10	OH	F	H	-214.87899	-214.22850	-214.89118	-214.24225
	11	SH	F	H	-537.79065	-537.14201	-537.80280	-537.15610
	12	Cl	Cl	H	-959.46903	-958.82192	-959.48161	-958.83639
	13	NH <sub>2</sub>	Cl	H	-555.27857	-554.63118	-555.28934	-554.64345
	14	OH	Cl	H	-575.15714	-574.51069	-575.16940	-574.52457
	15	SH	Cl	H	-898.07457	-897.43130	-898.08654	-897.44527
	16	NH <sub>2</sub>	NH <sub>2</sub>	H	-151.07036	-150.43100	-151.07889	-150.44120
	17	OH	NH <sub>2</sub>	H	-170.95724	-170.31243	-170.96732	-170.32421
	18	SH	NH <sub>2</sub>	H	-493.87378	-493.23800	-493.88377	-493.24981
	19	OH	OH	H	-190.84416	-190.19700	-190.85583	-190.21026
	20	SH	OH	H	-513.75801	-513.11352	-513.76962	-513.12699
	21	SH	SH	H	-836.67821	-836.03936	-836.68949	-836.05271
	22	F	F	F	-338.16589	-337.50262	-338.18388	-337.52213
	23	Cl	Cl	Cl	-1418.97998	-1418.33765	-1418.99833	-1418.35776
	24	NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	-206.39769	-205.75833	-206.40945	-205.77198
	25	OH	OH	OH	-266.06010	-265.41549	-266.07643	-265.43352
	26	SH	SH	SH	-1234.79637	-1234.16681	-1234.81258	-1234.18512
	27	NH <sub>2</sub>	F	OH	-270.21270	-269.56425	-270.22813	-269.58140
	28	SH	NH <sub>2</sub>	NH <sub>2</sub>	-549.19684	-548.56032	-549.21018	-548.57564
	29	SH	SH	NH <sub>2</sub>	-891.99668	-891.36523	-892.01153	-891.38195
{ $\pi_a$ }	30	BH <sub>2</sub>	H	H	-65.84123	-65.19676	-65.84313	-65.19967
	31	CHO	H	H	-153.71908	-153.07167	-153.72867	-153.08275
	32	CN	H	H	-132.65673	-132.00835	-132.66583	-132.01904
	33	COOH	H	H	-228.96023	-228.30840	-228.97474	-228.32456
	34	CHCH <sub>2</sub>	H	H	-117.76167	-117.12639	-117.76751	-117.13495
	35	CCH	H	H	-116.54331	-115.90269	-116.55048	-115.91199
	36	BH <sub>2</sub>	BH <sub>2</sub>	H	-91.24467	-90.60500	-91.24701	-90.60888
	37	BH <sub>2</sub>	CHO	H	-179.11988	-178.48155	-179.12986	-178.49242
	38	BH <sub>2</sub>	CN	H	-158.05555	-157.42125	-158.06495	-157.43187
	39	BH <sub>2</sub>	COOH	H	-254.36055	-253.71763	-254.37536	-253.73390
	40	CHO	CHO	H	-266.99240	-266.35560	-267.01010	-266.37414
	41	CHO	CN	H	-245.92785	-245.29249	-245.94513	-245.31080
	42	CHO	COOH	H	-342.23419	-341.59417	-342.25678	-341.61812
	43	CN	CN	H	-224.85629	-224.22166	-224.87318	-224.23963
	44	CN	COOH	H	-321.16647	-320.52739	-321.18869	-320.55102
	45	COOH	COOH	H	-417.47377	-416.83079	-417.50136	-416.86018

	46	CHCH <sub>2</sub>	BH <sub>2</sub>	H	-143.16064	-142.54178	-143.16701	-142.55004
	47	CHCH <sub>2</sub>	CHO	H	-231.03886	-230.41831	-231.05275	-230.43410
	48	CHCH <sub>2</sub>	CN	H	-209.97547	-209.35118	-209.98883	-209.36673
	49	CHCH <sub>2</sub>	COOH	H	-306.27937	-305.65307	-306.29815	-305.67408
	50	CHCH <sub>2</sub>	CHCH <sub>2</sub>	H	-195.08257	-194.46369	-195.09266	-194.47613
	51	CHCH <sub>2</sub>	CCH	H	-193.86261	-193.24338	-193.87402	-193.25707
	52	CCH	BH <sub>2</sub>	H	-141.94092	-141.31807	-141.94864	-141.32721
	53	CCH	CHO	H	-229.81820	-229.19180	-229.83345	-229.20851
	54	CCH	CN	H	-208.74950	-208.12201	-208.76432	-208.13836
	55	CCH	COOH	H	-305.05621	-304.42664	-305.07641	-304.44867
	56	CCH	CCH	H	-192.63887	-192.01671	-192.65170	-192.03130
	57	BH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-116.65860	-116.01915	-116.66156	-116.02389
	58	CHO	CHO	CHO	-380.26612	-379.63801	-380.29231	-379.66397
	59	CN	CN	CN	-317.04596	-316.42552	-317.07087	-316.45084
	60	CHCH <sub>2</sub>	CHCH <sub>2</sub>	CHCH <sub>2</sub>	-272.40392	-271.79429	-272.41822	-271.81005
	61	CCH	CCH	CCH	-268.73139	-268.12611	-268.74995	-268.14598
	62	CHO	CHO	CN	-359.19910	-358.57177	-359.22464	-358.59755
	63	CHCH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-168.56553	-167.94509	-168.57216	-167.95328
	64	CHCH <sub>2</sub>	BH <sub>2</sub>	CHCH <sub>2</sub>	-220.48447	-219.87440	-220.49520	-219.88645
	65	CCH	CCH	CN	-284.83997	-284.23073	-284.86057	-284.25250
	66	CCH	CHO	CN	-322.02150	-321.40500	-322.04458	-321.42892
{ $\pi_d\pi_aZ$ }	67	F	BH <sub>2</sub>	H	-165.06676	-164.43790	-165.07438	-164.44705
	68	F	CHO	H	-252.94532	-252.30784	-252.96053	-252.32477
	69	F	CN	H	-231.87517	-231.23309	-231.89007	-231.24969
	70	F	COOH	H	-328.18343	-327.54131	-328.20362	-327.56352
	71	F	CHCH <sub>2</sub>	H	-216.99238	-216.36254	-217.00378	-216.37681
	72	F	CCH	H	-215.76770	-215.13132	-215.78063	-215.14647
	73	Cl	BH <sub>2</sub>	H	-525.35530	-524.72508	-525.36264	-524.73416
	74	Cl	CHO	H	-613.23209	-612.59656	-613.24715	-612.61324
	75	Cl	CN	H	-592.16236	-591.52420	-592.17710	-591.54045
	76	Cl	COOH	H	-688.46903	-687.83036	-688.48905	-687.85240
	77	Cl	CHCH <sub>2</sub>	H	-577.27915	-576.64978	-577.29047	-576.66352
	78	Cl	CCH	H	-576.05452	-575.42143	-576.06732	-575.43612
	79	NH <sub>2</sub>	BH <sub>2</sub>	H	-121.16372	-120.54759	-121.16928	-120.55479
	80	NH <sub>2</sub>	CHO	H	-209.03178	-208.42072	-209.04476	-208.43523
	81	NH <sub>2</sub>	CN	H	-187.96557	-187.33957	-187.97818	-187.35382
	82	NH <sub>2</sub>	COOH	H	-284.27263	-283.65264	-284.29052	-283.67244
	83	NH <sub>2</sub>	CHCH <sub>2</sub>	H	-173.07346	-172.45712	-173.08269	-172.46858
	84	NH <sub>2</sub>	CCH	H	-171.85319	-171.23005	-171.86388	-171.24265
	85	OH	BH <sub>2</sub>	H	-141.03124	-140.41894	-141.03837	-140.42775
	86	OH	CHO	H	-228.91627	-228.29602	-228.93091	-228.31222
	87	OH	CN	H	-207.84443	-207.21278	-207.85871	-207.22875
	88	OH	COOH	H	-304.15614	-303.52823	-304.17563	-303.54973
	89	OH	CHCH <sub>2</sub>	H	-192.95674	-192.33577	-192.96759	-192.34905
	90	OH	CCH	H	-191.73437	-191.10805	-191.74671	-191.12245
	91	SH	BH <sub>2</sub>	H	-463.96803	-463.34169	-463.97516	-463.35039
	92	SH	CHO	H	-551.83770	-551.21507	-551.85217	-551.23114
	93	SH	CN	H	-530.76951	-530.13885	-530.78356	-530.15447
	94	SH	COOH	H	-627.07579	-626.44891	-627.09511	-626.47031
	95	SH	CHCH <sub>2</sub>	H	-515.88231	-515.25606	-515.89299	-515.26917
	96	SH	CCH	H	-514.65918	-514.03241	-514.67127	-514.04634
	97	NH <sub>2</sub>	BH <sub>2</sub>	OH	-196.37010	-195.76639	-196.38085	-195.77860
	98	NH <sub>2</sub>	BH <sub>2</sub>	F	-220.39930	-219.78971	-220.41057	-219.80254

	99	NH <sub>2</sub>	BH <sub>2</sub>	NH <sub>2</sub>	-176.48770	-175.88218	-176.49679	-175.89274
	100	NH <sub>2</sub>	BH <sub>2</sub>	CHO	-234.45763	-233.84380	-234.47131	-233.85889
	101	NH <sub>2</sub>	BH <sub>2</sub>	COOH	-309.69584	-309.07704	-309.71429	-309.09719
	102	NH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-146.58400	-145.96113	-146.59018	-145.96873
	103	NH <sub>2</sub>	BH <sub>2</sub>	CN	-213.38255	-212.76876	-213.39583	-212.78346
	104	NH <sub>2</sub>	BH <sub>2</sub>	CCH	-197.27119	-196.66102	-197.28253	-196.67380
	105	NH <sub>2</sub>	BH <sub>2</sub>	CHCH <sub>2</sub>	-198.49145	-197.88298	-198.50141	-197.89425
	106	NH <sub>2</sub>	CHO	OH	-284.23895	-283.63600	-284.25696	-283.65545
	107	NH <sub>2</sub>	CHO	F	-308.27278	-307.65584	-308.29147	-307.67583
	108	NH <sub>2</sub>	CHO	NH <sub>2</sub>	-264.35261	-263.75129	-264.36898	-263.76905
	109	NH <sub>2</sub>	CHO	CHO	-322.31141	-321.71762	-322.33251	-321.74001
	110	NH <sub>2</sub>	CHO	COOH	-397.55369	-396.95188	-397.57985	-396.97945
	111	NH <sub>2</sub>	CHO	CN	-301.24023	-300.64043	-301.26091	-300.66252
	112	NH <sub>2</sub>	CHO	CCH	-285.13186	-284.53460	-285.15052	-284.55471
	113	NH <sub>2</sub>	CHO	CHCH <sub>2</sub>	-286.35448	-285.75540	-286.37174	-285.77414
	114	OH	BH <sub>2</sub>	OH	-216.23932	-215.64258	-216.25228	-215.65638
	115	OH	BH <sub>2</sub>	BH <sub>2</sub>	-166.43995	-165.82700	-166.44818	-165.83617
	116	OH	BH <sub>2</sub>	CCH	-217.13260	-216.53182	-217.14615	-216.54623
	117	OH	CHO	OH	-304.12390	-303.51355	-304.14358	-303.53454
	118	OH	CHO	CHO	-342.19591	-341.58187	-342.21864	-341.60564
	119	OH	CHO	CCH	-305.01549	-304.40999	-305.03584	-304.43178
	120	F	BH <sub>2</sub>	F	-264.30065	-263.68832	-264.31395	-263.70327
	121	F	BH <sub>2</sub>	BH <sub>2</sub>	-190.47158	-189.84569	-190.47973	-189.85509
	122	F	BH <sub>2</sub>	CN	-257.27367	-256.65381	-257.28897	-256.67045
	123	NH <sub>2</sub>	CCH	NH <sub>2</sub>	-227.17052	-226.55554	-227.18466	-226.57113
	124	NH <sub>2</sub>	CCH	CCH	-247.94817	-247.34505	-247.96450	-247.36295
	125	F	CHO	CCH	-329.04378	-328.42171	-329.06486	-328.44410
	126	NH <sub>2</sub>	CN	F	-287.20433	-286.56699	-287.22275	-286.58697
	127	NH <sub>2</sub>	CN	CN	-280.16394	-279.55595	-280.18430	-279.57766
{CQ <sub>3</sub> }	128	CH <sub>3</sub>	H	H	-79.70279	-79.04802	-79.70585	-79.05265
	129	CF <sub>3</sub>	H	H	-377.44273	-376.78012	-377.46247	-376.80108
	130	CH <sub>3</sub>	CH <sub>3</sub>	H	-118.96563	-118.31568	-118.97010	-118.32193
	131	CF <sub>3</sub>	CF <sub>3</sub>	H	-714.43363	-713.77123	-714.47068	-713.81027
	132	CF <sub>3</sub>	CH <sub>3</sub>	H	-416.70634	-416.05084	-416.72704	-416.07344
	133	CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	-158.23098	-157.58436	-158.23683	-157.59213
	134	CF <sub>3</sub>	CF <sub>3</sub>	CF <sub>3</sub>	-1051.41508	-1050.75539	-1051.46979	-1050.81238
{X-CQ <sub>3</sub> }	135	F	CH <sub>3</sub>	H	-178.93681	-178.28516	-178.94542	-178.29550
	136	Cl	CH <sub>3</sub>	H	-539.22254	-538.57352	-539.23096	-538.58383
	137	NH <sub>2</sub>	CH <sub>3</sub>	H	-135.01533	-134.37600	-135.02183	-134.38429
	138	OH	CH <sub>3</sub>	H	-154.89985	-154.25535	-154.90792	-154.26521
	139	SH	CH <sub>3</sub>	H	-477.82267	-477.17993	-477.83047	-477.18981
	140	F	CF <sub>3</sub>	H	-476.66503	-476.00826	-476.68997	-476.03513
	141	Cl	CF <sub>3</sub>	H	-836.95167	-836.29944	-836.97640	-836.32631
	142	NH <sub>2</sub>	CF <sub>3</sub>	H	-432.75517	-432.11238	-432.77788	-432.13735
	143	OH	CF <sub>3</sub>	H	-452.63444	-451.98676	-452.65880	-452.01327
	144	SH	CF <sub>3</sub>	H	-775.55806	-774.91253	-775.58214	-774.93901
	145	NH <sub>2</sub>	F	CH <sub>3</sub>	-234.26889	-233.61924	-234.28093	-233.63294
	146	NH <sub>2</sub>	NH <sub>2</sub>	CF <sub>3</sub>	-488.07520	-487.43848	-488.10116	-487.46670
	147	NH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	-769.74705	-769.10905	-769.78738	-769.15187
	148	BH <sub>2</sub>	CH <sub>3</sub>	H	-105.10050	-104.46685	-105.10390	-104.47154
	149	CHO	CH <sub>3</sub>	H	-192.98241	-192.34466	-192.99341	-192.35720
	150	CN	CH <sub>3</sub>	H	-171.91893	-171.27774	-171.92949	-171.28993

151	COOH	CH <sub>3</sub>	H	-268.22177	-267.58090	-268.23771	-267.59863
152	CHCH <sub>2</sub>	CH <sub>3</sub>	H	-157.02418	-156.39363	-157.03146	-156.40346
153	CCH	CH <sub>3</sub>	H	-155.80540	-155.17043	-155.81402	-155.18117
154	BH <sub>2</sub>	CF <sub>3</sub>	H	-402.84222	-402.19376	-402.86181	-402.21474
155	CHO	CF <sub>3</sub>	H	-490.71455	-490.06288	-490.74192	-490.09179
156	CN	CF <sub>3</sub>	H	-469.64741	-468.99834	-469.67438	-469.02697
157	COOH	CF <sub>3</sub>	H	-565.95327	-565.30045	-565.98559	-565.33462
158	CHCH <sub>2</sub>	CF <sub>3</sub>	H	-454.76271	-454.12746	-454.78625	-454.15380
159	CCH	CF <sub>3</sub>	H	-453.53941	-452.89873	-453.56435	-452.92587
160	BH <sub>2</sub>	CN	CH <sub>3</sub>	-197.31477	-196.69230	-197.32571	-196.70445
161	BH <sub>2</sub>	BH <sub>2</sub>	CF <sub>3</sub>	-428.24646	-427.60184	-428.26640	-427.62365
162	BH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	-739.83130	-739.18324	-739.86854	-739.22233
163	NH <sub>2</sub>	BH <sub>2</sub>	CH <sub>3</sub>	-160.43075	-159.81727	-160.43778	-159.82588
164	NH <sub>2</sub>	CHO	CH <sub>3</sub>	-248.29855	-247.69226	-248.31293	-247.70814
165	NH <sub>2</sub>	BH <sub>2</sub>	CF <sub>3</sub>	-458.16793	-457.54655	-458.19124	-457.57169
166	NH <sub>2</sub>	CHO	CF <sub>3</sub>	-546.02902	-545.41688	-546.05968	-545.44937

<sup>a</sup> Including scaled (by 0.9806) UB3-LYP/6-31G(d) ZPVEs; <sup>b</sup> Energy calculations carried out with the 6-311+G(3df,2p) basis set on UB3-LYP/6-31G(d) geometries.

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**Table S3** G3X(MP2)-RAD energies of substituted methanes (CHXYZ) and substituted radicals ( $\bullet$ CXYZ) (0 K, Hartrees).

X	Y	Z	E(CHXYZ)	E( $\bullet$ CXYZ)
CH <sub>3</sub>	C $\equiv$ CH	H	-155.67836	-155.03787
CH <sub>3</sub>	CH <sub>3</sub>	H	-118.88479	-118.22897
CH <sub>3</sub>	CH=CH <sub>2</sub>	H	-156.90653	-156.27030
CH <sub>3</sub>	CHO	H	-192.83502	-192.19150
CH <sub>3</sub>	Cl	H	-538.81231	-538.15783
CH <sub>3</sub>	CN	H	-171.78067	-171.13345
CH <sub>3</sub>	F	H	-178.81056	-178.15301
CH <sub>3</sub>	OH	H	-154.79186	-154.14116
CH=CH <sub>2</sub>	CH=CH <sub>2</sub>	H	-194.92826	-194.30494
Cl	CF <sub>3</sub>	H	-836.32085	-835.66178
Cl	Cl	H	-958.73081	-958.07808
CN	CN	H	-224.66145	-224.02022
COOH	Cl	H	-687.93544	-687.29063
COOH	CN	H	-320.90486	-320.25944
COOH	COOH	H	-417.14506	-416.49669
COOH	NH <sub>2</sub>	H	-284.05675	-283.42785
F	F	H	-238.74051	-238.07865
NH <sub>2</sub>	CN	H	-187.81600	-187.18197
OH	CH=CH <sub>2</sub>	H	-192.81218	-192.18636
F	Cl	H	-598.73195	-598.07422
BH <sub>2</sub>	BH <sub>2</sub>	H	-91.15425	-90.50789
CF <sub>3</sub>	BH <sub>2</sub>	H	-402.53532	-401.88036
CF <sub>3</sub>	CF <sub>3</sub>	H	-713.91042	-713.24212
CH <sub>3</sub>	BH <sub>2</sub>	H	-105.01465	-104.37461
CH <sub>3</sub>	CF <sub>3</sub>	H	-416.40428	-415.74242
CH <sub>3</sub>	CH <sub>3</sub>	H	-118.88479	-118.22897
CH <sub>3</sub>	NH <sub>2</sub>	H	-134.92319	-134.27724
NH <sub>2</sub>	BH <sub>2</sub>	H	-121.06770	-120.44252
NH <sub>2</sub>	CF <sub>3</sub>	H	-432.44160	-431.79107
NH <sub>2</sub>	NH <sub>2</sub>	H	-150.96684	-150.32047
F	CH=CH <sub>2</sub>	H	-216.82933	-216.19589
Cl	CH=CH <sub>2</sub>	H	-576.83212	-576.19906
BH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	-739.27598	-738.62057
BH <sub>2</sub>	BH <sub>2</sub>	CF <sub>3</sub>	-427.90693	-427.25476
BH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-116.53618	-115.88838
NH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-146.45519	-145.82174
NH <sub>2</sub>	CF <sub>3</sub>	BH <sub>2</sub>	-457.82217	-457.19135
NH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	-769.18484	-768.53766
NH <sub>2</sub>	NH <sub>2</sub>	BH <sub>2</sub>	-176.35119	-175.73670
NH <sub>2</sub>	NH <sub>2</sub>	CF <sub>3</sub>	-487.72254	-487.07703
NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	-206.25493	-205.60725
CN	BH <sub>2</sub>	CH <sub>3</sub>	-197.14287	-196.51314
CN	CN	CN	-316.76649	-316.13780
F	BH <sub>2</sub>	BH <sub>2</sub>	-190.30666	-189.67381
F	BH <sub>2</sub>	BH <sub>2</sub>	-190.30666	-189.67381

F	BH <sub>2</sub>	F	-264.09658	-263.47674
F	F	F	-337.92164	-337.25144
NH <sub>2</sub>	BH <sub>2</sub>	CH <sub>3</sub>	-160.30604	-159.68351
NH <sub>2</sub>	BH <sub>2</sub>	CN	-213.19936	-212.57597
NH <sub>2</sub>	BH <sub>2</sub>	F	-220.22899	-219.61043
NH <sub>2</sub>	F	CH <sub>3</sub>	-234.10252	-233.44550
NH <sub>2</sub>	F	CN	-286.98026	-286.33465
C≡CH	C≡CH	C≡CH	-268.48432	-267.87036
C≡CH	C≡CH	CN	-284.58189	-283.96411
CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	-158.12227	-157.46857
CHO	C≡CH	CN	-321.74300	-321.11858
CHO	CHO	CHO	-379.95789	-379.32477
CHO	CHO	CN	-358.90047	-358.26612
Cl	Cl	Cl	-1417.88561	-1417.23673
F	CHO	C≡CH	-328.77698	-328.14653
NH <sub>2</sub>	C≡CH	CCH	-247.73587	-247.12326
NH <sub>2</sub>	C≡CH	NH <sub>2</sub>	-226.99292	-226.36877
NH <sub>2</sub>	CHO	C≡CH	-284.89933	-284.29112
NH <sub>2</sub>	CHO	NH <sub>2</sub>	-264.15452	-263.54142
NH <sub>2</sub>	CN	CN	-279.92959	-279.31120
NH <sub>2</sub>	F	OH	-270.01948	-269.36320
OH	OH	OH	-265.86905	-265.21714
CH=CH <sub>2</sub>	CH=CH <sub>2</sub>	CH=CH <sub>2</sub>	-272.18575	-271.57034
NH <sub>2</sub>	BH <sub>2</sub>	C≡CH	-197.09963	-196.47953
NH <sub>2</sub>	CHO	BH <sub>2</sub>	-234.26568	-233.64218
NH <sub>2</sub>	CHO	CF <sub>3</sub>	-545.62196	-544.99862
NH <sub>2</sub>	CHO	CH <sub>3</sub>	-248.11184	-247.49513
NH <sub>2</sub>	CHO	CH=CH <sub>2</sub>	-286.13161	-285.52220
NH <sub>2</sub>	CHO	CHO	-322.05750	-321.45249
NH <sub>2</sub>	CHO	CN	-300.99658	-300.38548
NH <sub>2</sub>	CHO	F	-308.03952	-307.41250
NH <sub>2</sub>	CHO	OH	-284.02477	-283.41003
NH <sub>2</sub>	BH <sub>2</sub>	CH=CH <sub>2</sub>	-198.32944	-197.71257
NH <sub>2</sub>	BH <sub>2</sub>	OH	-196.21823	-195.60535
OH	BH <sub>2</sub>	BH <sub>2</sub>	-166.29533	-165.67277
OH	BH <sub>2</sub>	C≡CH	-216.94538	-216.33625
OH	BH <sub>2</sub>	OH	-216.07184	-215.46600
OH	CHO	C≡CH	-304.76690	-304.15171
OH	CHO	CHO	-341.92626	-341.30319
OH	CHO	OH	-303.89416	-303.27264
NH <sub>2</sub>	BH <sub>2</sub>	COOH	-309.44702	-308.81878
NH <sub>2</sub>	CHO	COOH	-397.24339	-396.63036
SH	NH <sub>2</sub>	NH <sub>2</sub>	-548.73005	-548.08569
SH	SH	NH <sub>2</sub>	-891.21087	-890.56808
SH	SH	SH	-1233.68400	-1233.04836
CH=CH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	-168.40975	-167.78255
CH=CH <sub>2</sub>	BH <sub>2</sub>	CH=CH <sub>2</sub>	-220.29735	-219.68102



**Table S4** Calculated bond dissociation energies (BDEs), radical stabilization energies (RSEs), molecule interaction energies (MIEs), radical interaction energies (RIEs), deviations from additivity of RSEs (DARSEs), pairwise MIEs (PMIEs), pairwise RIEs (PRIEs), and deviations from pairwise additivity of RSEs (DPARSEs) (0 K, kJ mol<sup>-1</sup>) for the { $\pi_d$ }, { $\pi_a$ }, { $\pi_d\pi_aZ$ }, {CQ<sub>3</sub>}, and {X-CQ<sub>3</sub>} sets

Set	#	X	Y	Z	BDE <sup>a</sup>	RSE <sup>a</sup>	MIE <sup>a</sup>	RIE <sup>a</sup>	DARSE <sup>a</sup>	PMIE <sup>a</sup>	PRIE <sup>a</sup>	DPARSE <sup>a</sup>
{ $\pi_d$ }	1	H	H	H	423.5	0.0						
	2	F	H	H	407.3	16.2						
	3	Cl	H	H	399.0	24.5						
	4	NH <sub>2</sub>	H	H	371.4	52.1						
	5	OH	H	H	386.3	37.2						
	6	SH	H	H	382.0	41.5						
	7	F	F	H	408.0	15.5	52.7	35.9	-16.9			
	8	Cl	F	H	397.8	25.6	21.0	6.0	-15.0			
	9	NH <sub>2</sub>	F	H	399.2	24.3	64.1	20.1	-43.9			
	10	OH	F	H	394.7	28.8	61.7	37.2	-24.5			
	11	SH	F	H	388.8	34.7	22.2	-0.8	-23.0			
	12	Cl	Cl	H	384.9	38.6	3.6	-6.8	-10.3			
	13	NH <sub>2</sub>	Cl	H	386.7	36.8	45.3	5.6	-39.7			
	14	OH	Cl	H	383.9	39.6	35.3	13.3	-22.0			
	15	SH	Cl	H	374.6	48.9	10.3	-6.7	-17.0			
	16	NH <sub>2</sub>	NH <sub>2</sub>	H	365.2	58.3	39.3	-6.5	-45.9			
	17	OH	NH <sub>2</sub>	H	379.4	44.1	51.4	6.2	-45.2			
	18	SH	NH <sub>2</sub>	H	355.3	68.1	24.5	-0.9	-25.4			
	19	OH	OH	H	385.8	37.7	63.6	26.9	-36.7			
	20	SH	OH	H	378.1	45.4	29.7	-3.5	-33.3			
	21	SH	SH	H	362.8	60.7	11.8	-10.4	-22.2			
	22	F	F	F	428.3	-4.8	134.1	80.8	-53.4	-24.0	-26.8	-2.8
	23	Cl	Cl	Cl	372.7	50.8	1.9	-20.8	-22.7	-8.8	-0.3	8.4
	24	NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	364.6	58.9	95.5	-1.9	-97.4	-22.5	17.6	40.2
	25	OH	OH	OH	378.9	44.6	136.0	69.1	-66.9	-54.7	-11.6	43.2
	26	SH	SH	SH	338.3	85.2	20.7	-18.5	-39.2	-14.7	12.7	27.4
	27	NH <sub>2</sub>	F	OH	388.9	34.6	134.7	63.8	-70.8	-42.5	0.3	42.8
	28	SH	NH <sub>2</sub>	NH <sub>2</sub>	356.9	66.6	69.7	-9.3	-79.0	-18.5	-0.9	17.6
	29	SH	SH	NH <sub>2</sub>	343.9	79.6	45.6	-9.8	-55.4	-15.1	2.5	17.6
{ $\pi_a$ }	30	BH <sub>2</sub>	H	H	380.3	43.2						
	31	CHO	H	H	386.7	36.8						
	32	CN	H	H	389.0	34.5						
	33	COOH	H	H	397.9	25.6						
	34	CHCH <sub>2</sub>	H	H	351.7	71.9						
	35	CCH	H	H	367.2	56.3						
	36	BH <sub>2</sub>	BH <sub>2</sub>	H	366.3	57.2	16.5	-12.7	-29.2			
	37	BH <sub>2</sub>	CHO	H	364.5	59.0	9.5	-11.5	-20.9			
	38	BH <sub>2</sub>	CN	H	353.0	70.4	4.1	-3.1	-7.2			
	39	BH <sub>2</sub>	COOH	H	375.0	48.4	8.0	-12.3	-20.3			
	40	CHO	CHO	H	360.6	62.9	-4.4	-15.1	-10.6			
	41	CHO	CN	H	356.3	67.2	-10.0	-14.0	-4.0			

	42	CHO	COOH	H	367.7	55.8	-2.8	-9.3	-6.5			
	43	CN	CN	H	354.3	69.2	-33.9	-33.6	0.3			
	44	CN	COOH	H	365.1	58.4	-16.6	-18.2	-1.6			
	45	COOH	COOH	H	374.3	49.2	-6.8	-8.7	-1.9			
	46	CHCH <sub>2</sub>	BH <sub>2</sub>	H	310.7	112.8	5.0	2.8	-2.3			
	47	CHCH <sub>2</sub>	CHO	H	315.1	108.3	5.6	5.3	-0.2			
	48	CHCH <sub>2</sub>	CN	H	324.2	99.3	2.7	-4.3	-7.0			
	49	CHCH <sub>2</sub>	COOH	H	329.4	94.1	3.8	0.5	-3.3			
	50	CHCH <sub>2</sub>	CHCH <sub>2</sub>	H	309.6	113.9	8.4	-21.3	-29.7			
	51	CHCH <sub>2</sub>	CCH	H	310.7	112.8	4.2	-11.1	-15.3			
	52	CCH	BH <sub>2</sub>	H	322.5	101.0	1.5	3.1	1.6			
	53	CCH	CHO	H	331.7	91.8	-0.4	-1.5	-1.2			
	54	CCH	CN	H	334.3	89.1	-16.9	-18.4	-1.5			
	55	CCH	COOH	H	339.0	84.5	-8.6	-5.9	2.7			
	56	CCH	CCH	H	319.7	103.7	-9.7	-18.5	-8.7			
	57	BH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	365.1	58.4	61.1	-10.1	-71.2	11.5	27.9	16.4
	58	CHO	CHO	CHO	340.6	82.9	-6.8	-34.2	-27.3	6.4	11.0	4.5
	59	CN	CN	CN	318.8	104.7	-93.2	-91.9	1.4	8.5	9.0	0.5
	60	CHCH <sub>2</sub>	CHCH <sub>2</sub>	CHCH <sub>2</sub>	287.6	135.9	17.8	-61.8	-79.6	-7.3	2.3	9.5
	61	CCH	CCH	CCH	276.6	146.9	-27.3	-49.1	-21.8	2.0	6.3	4.3
	62	CHO	CHO	CN	337.3	86.2	-19.5	-41.3	-21.8	5.0	1.9	-3.1
	63	CHCH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	315.7	107.7	24.9	-25.6	-50.5	-1.7	-18.5	-16.8
	64	CHCH <sub>2</sub>	BH <sub>2</sub>	CHCH <sub>2</sub>	289.1	134.3	21.4	-31.1	-52.5	3.0	-15.3	-18.3
	65	CCH	CCH	CN	287.4	136.1	-39.7	-50.5	-10.8	3.9	4.9	1.0
	66	CCH	CHO	CN	307.3	116.2	-24.4	-35.6	-11.3	2.9	-1.6	-4.5
{ $\pi_a\pi_aZ$ }	67	F	BH <sub>2</sub>	H	337.9	85.5	5.7	31.9	26.2			
	68	F	CHO	H	360.1	63.4	7.3	17.8	10.5			
	69	F	CN	H	372.2	51.3	-12.7	-12.1	0.6			
	70	F	COOH	H	371.5	52.0	-0.5	9.8	10.3			
	71	F	CHCH <sub>2</sub>	H	337.0	86.5	18.9	17.4	-1.5			
	72	F	CCH	H	355.9	67.6	2.8	-2.0	-4.8			
	73	Cl	BH <sub>2</sub>	H	341.0	82.5	5.7	20.5	14.9			
	74	Cl	CHO	H	355.2	68.2	3.0	10.0	7.1			
	75	Cl	CN	H	362.4	61.1	-16.0	-13.8	2.2			
	76	Cl	COOH	H	362.4	61.1	-8.0	3.0	11.0			
	77	Cl	CHCH <sub>2</sub>	H	337.0	86.5	14.7	5.0	-9.7			
	78	Cl	CCH	H	348.1	75.4	-1.3	-6.7	-5.3			
	79	NH <sub>2</sub>	BH <sub>2</sub>	H	304.2	119.2	44.6	68.5	24.0			
	80	NH <sub>2</sub>	CHO	H	291.2	132.3	18.2	61.6	43.4			
	81	NH <sub>2</sub>	CN	H	330.1	93.3	8.3	15.1	6.8			
	82	NH <sub>2</sub>	COOH	H	313.7	109.8	17.3	49.5	32.2			
	83	NH <sub>2</sub>	CHCH <sub>2</sub>	H	303.2	120.2	15.8	12.1	-3.7			
	84	NH <sub>2</sub>	CCH	H	321.9	101.6	11.1	4.3	-6.8			
	85	OH	BH <sub>2</sub>	H	294.1	129.4	5.8	54.8	49.0			
	86	OH	CHO	H	315.3	108.2	24.2	58.5	34.3			
	87	OH	CN	H	344.8	78.6	-0.4	6.6	7.0			
	88	OH	COOH	H	334.2	89.3	20.6	47.2	26.6			
	89	OH	CHCH <sub>2</sub>	H	314.9	108.6	18.5	18.1	-0.4			
	90	OH	CCH	H	329.9	93.6	8.4	8.6	0.2			
	91	SH	BH <sub>2</sub>	H	331.2	92.3	32.3	39.9	7.6			
	92	SH	CHO	H	321.4	102.1	9.9	33.8	23.9			
	93	SH	CN	H	342.6	80.9	-5.2	-0.2	5.0			
	94	SH	COOH	H	331.3	92.2	1.7	26.9	25.2			

	95	SH	CHCH <sub>2</sub>	H	328.7	94.7	15.1	-3.4	-18.5			
	96	SH	CCH	H	331.6	91.8	2.8	-3.1	-5.9			
	97	NH <sub>2</sub>	BH <sub>2</sub>	OH	272.1	151.4	93.2	112.2	18.9	-8.5	-17.4	-8.9
	98	NH <sub>2</sub>	BH <sub>2</sub>	F	287.3	136.2	76.6	101.4	24.8	-37.7	-19.2	18.6
	99	NH <sub>2</sub>	BH <sub>2</sub>	NH <sub>2</sub>	276.8	146.7	92.7	92.0	-0.7	-35.8	-38.6	-2.8
	100	NH <sub>2</sub>	BH <sub>2</sub>	CHO	298.8	124.7	94.2	86.9	-7.3	22.0	-31.8	-53.8
	101	NH <sub>2</sub>	BH <sub>2</sub>	COOH	311.1	112.4	86.1	77.6	-8.4	16.2	-28.1	-44.3
	102	NH <sub>2</sub>	BH <sub>2</sub>	BH <sub>2</sub>	322.5	101.0	105.8	68.3	-37.5	0.1	-56.1	-56.2
	103	NH <sub>2</sub>	BH <sub>2</sub>	CN	298.7	124.8	61.0	56.1	-4.9	4.1	-24.4	-28.5
	104	NH <sub>2</sub>	BH <sub>2</sub>	CCH	289.1	134.4	66.4	49.2	-17.1	9.2	-26.7	-35.9
	105	NH <sub>2</sub>	BH <sub>2</sub>	CHCH <sub>2</sub>	285.0	138.5	71.2	42.7	-28.6	5.9	-40.7	-46.6
	106	NH <sub>2</sub>	CHO	OH	270.1	153.3	68.5	95.8	27.3	-25.2	-30.5	-5.2
	107	NH <sub>2</sub>	CHO	F	307.2	116.2	64.4	75.6	11.2	-25.1	-23.9	1.3
	108	NH <sub>2</sub>	CHO	NH <sub>2</sub>	266.0	157.5	57.6	74.2	16.6	-18.0	-42.5	-24.5
	109	NH <sub>2</sub>	CHO	CHO	246.5	177.0	30.3	81.7	51.4	-1.6	-26.4	-24.8
	110	NH <sub>2</sub>	CHO	COOH	267.3	156.2	33.6	75.5	41.8	1.0	-26.3	-27.3
	111	NH <sub>2</sub>	CHO	CN	262.0	161.5	7.3	45.6	38.3	-9.2	-17.1	-8.0
	112	NH <sub>2</sub>	CHO	CCH	255.2	168.3	20.3	43.5	23.2	-8.5	-20.8	-12.3
	113	NH <sub>2</sub>	CHO	CHCH <sub>2</sub>	259.9	163.6	31.3	34.3	2.9	-8.1	-44.7	-36.6
	114	OH	BH <sub>2</sub>	OH	255.4	168.0	60.6	111.1	50.5	-14.5	-25.4	-10.9
	115	OH	BH <sub>2</sub>	BH <sub>2</sub>	297.7	125.7	37.9	40.1	2.2	9.8	-56.9	-66.7
	116	OH	BH <sub>2</sub>	CCH	266.0	157.5	13.3	34.2	20.9	-2.4	-32.4	-29.9
	117	OH	CHO	OH	289.9	133.5	75.7	98.2	22.5	-36.2	-45.6	-9.5
	118	OH	CHO	CHO	300.3	123.2	36.3	48.8	12.5	-7.6	-53.1	-45.5
	119	OH	CHO	CCH	276.8	146.6	24.2	40.7	16.5	-8.0	-24.9	-16.8
	120	F	BH <sub>2</sub>	F	294.2	129.3	33.2	86.9	53.7	-30.9	-12.6	18.2
	121	F	BH <sub>2</sub>	BH <sub>2</sub>	330.9	92.6	26.1	16.1	-10.0	-1.8	-34.9	-33.1
	122	F	BH <sub>2</sub>	CN	314.8	108.7	-9.2	5.6	14.8	-6.3	-11.1	-4.8
	123	NH <sub>2</sub>	CCH	NH <sub>2</sub>	301.7	121.8	41.5	2.9	-38.7	-19.9	0.8	20.7
	124	NH <sub>2</sub>	CCH	CCH	270.3	153.2	-0.2	-11.6	-11.3	-12.6	-1.7	10.9
	125	F	CHO	CCH	320.7	102.8	5.7	-0.6	-6.4	-4.0	-14.9	-10.9
	126	NH <sub>2</sub>	CN	F	360.1	63.3	49.0	9.6	-39.4	-10.7	-13.6	-2.9
	127	NH <sub>2</sub>	CN	CN	283.6	139.9	-28.8	-10.0	18.9	-11.6	-6.6	5.0
{CQ <sub>3</sub> }	128	CH <sub>3</sub>	H	H	405.8	17.7						
	129	CF <sub>3</sub>	H	H	427.4	-3.8						
	130	CH <sub>3</sub>	CH <sub>3</sub>	H	392.6	30.8	10.4	6.0	-4.5			
	131	CF <sub>3</sub>	CF <sub>3</sub>	H	424.8	-1.3	-22.9	-16.4	6.4			
	132	CF <sub>3</sub>	CH <sub>3</sub>	H	406.9	16.6	11.2	14.0	2.7			
	133	CH <sub>3</sub>	CH <sub>3</sub>	CH <sub>3</sub>	383.6	39.9	27.3	14.3	-13.0	-3.9	-3.6	0.3
	134	CF <sub>3</sub>	CF <sub>3</sub>	CF <sub>3</sub>	416.9	6.6	-69.6	-51.4	18.2	-1.0	-2.1	-1.1
{X-CQ <sub>3</sub> }	135	F	CH <sub>3</sub>	H	397.3	26.2	27.6	20.0	-7.7			
	136	Cl	CH <sub>3</sub>	H	389.9	33.6	20.4	11.8	-8.7			
	137	NH <sub>2</sub>	CH <sub>3</sub>	H	364.7	58.7	17.9	6.9	-11.1			
	138	OH	CH <sub>3</sub>	H	378.3	45.1	23.7	14.1	-9.8			
	139	SH	CH <sub>3</sub>	H	373.0	50.5	12.9	4.3	-8.7			
	140	F	CF <sub>3</sub>	H	410.2	13.3	-4.1	-3.1	1.0			
	141	Cl	CF <sub>3</sub>	H	397.7	25.8	-9.0	-3.8	5.2			
	142	NH <sub>2</sub>	CF <sub>3</sub>	H	372.6	50.9	16.4	19.0	2.7			
	143	OH	CF <sub>3</sub>	H	385.7	37.8	8.7	13.1	4.5			
	144	SH	CF <sub>3</sub>	H	379.4	44.0	-0.1	6.3	6.5			
	145	NH <sub>2</sub>	F	CH <sub>3</sub>	392.2	31.3	96.7	42.1	-54.6	-12.8	-4.9	7.9
	146	NH <sub>2</sub>	NH <sub>2</sub>	CF <sub>3</sub>	356.7	66.8	53.4	19.9	-33.5	-18.7	-11.7	7.0

147	NH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	359.4	64.0	-3.1	16.6	19.7	-13.0	-5.0	7.9
148	BH <sub>2</sub>	CH <sub>3</sub>	H	351.1	72.3	1.2	12.8	11.4			
149	CHO	CH <sub>3</sub>	H	361.2	62.2	11.7	19.5	7.8			
150	CN	CH <sub>3</sub>	H	370.0	53.4	8.8	10.2	1.3			
151	COOH	CH <sub>3</sub>	H	368.8	54.7	7.0	18.5	11.5			
152	CHCH <sub>2</sub>	CH <sub>3</sub>	H	339.7	83.8	9.6	3.9	-5.8			
153	CCH	CH <sub>3</sub>	H	352.4	71.0	8.5	5.7	-2.9			
154	BH <sub>2</sub>	CF <sub>3</sub>	H	389.8	33.7	4.6	-1.0	-5.6			
155	CHO	CF <sub>3</sub>	H	397.8	25.7	-9.6	-16.8	-7.2			
156	CN	CF <sub>3</sub>	H	390.6	32.8	-22.0	-19.7	2.3			
157	COOH	CF <sub>3</sub>	H	400.0	23.5	-15.9	-14.1	1.8			
158	CHCH <sub>2</sub>	CF <sub>3</sub>	H	351.4	72.1	4.8	8.9	4.2			
159	CCH	CF <sub>3</sub>	H	367.2	56.3	-8.0	-4.1	3.9			
160	BH <sub>2</sub>	CN	CH <sub>3</sub>	322.0	101.5	5.3	11.5	6.2	-8.9	-8.3	0.5
161	BH <sub>2</sub>	BH <sub>2</sub>	CF <sub>3</sub>	378.4	45.1	23.0	-14.4	-37.4	-2.7	0.2	2.9
162	BH <sub>2</sub>	CF <sub>3</sub>	CF <sub>3</sub>	387.5	36.0	-22.2	-21.6	0.5	-8.5	-3.2	5.3
163	NH <sub>2</sub>	BH <sub>2</sub>	CH <sub>3</sub>	297.4	126.0	66.1	79.2	13.1	2.4	-8.9	-11.4
164	NH <sub>2</sub>	CHO	CH <sub>3</sub>	278.8	144.7	38.8	77.1	38.3	-8.9	-10.9	-2.1
165	NH <sub>2</sub>	BH <sub>2</sub>	CF <sub>3</sub>	317.5	106.0	57.8	72.3	14.6	-7.8	-14.2	-6.5
166	NH <sub>2</sub>	CHO	CF <sub>3</sub>	293.3	130.2	12.9	58.2	45.3	-12.0	-5.6	6.4

<sup>a</sup> Calculated at the UB2-PLYP/6-311+G(3df,2p)//UB3-LYP/6-31G(d) level.

**Table S5** Optimized UB3-LYP/6-31G(d) geometries of di- (CH<sub>2</sub>XY) and tri- (CHXYZ) substituted methanes

**(CH<sub>3</sub>, BH<sub>2</sub>, H)**

6	-1.226984	0.230847	-0.022378
1	-1.359477	0.740907	-0.983627
1	-1.277288	0.997081	0.759702
1	-2.082319	-0.441778	0.112830
5	1.429964	0.314616	-0.023570
1	1.434329	1.502930	0.141113
1	2.482607	-0.238321	-0.177623
6	0.111816	-0.520222	0.023899
1	0.201164	-1.071991	0.982364
1	0.142171	-1.325662	-0.726037

**(CH<sub>3</sub>, CCH, H)**

6	-0.740375	-0.415384	0.000000
6	-1.334198	-1.467121	0.000000
1	-1.862237	-2.393280	0.000000
6	0.000000	0.847983	0.000000
6	1.527616	0.651590	0.000000
1	-0.294333	1.440196	0.877236
1	-0.294333	1.440196	-0.877236
1	2.034970	1.622332	0.000000
1	1.848836	0.094075	0.885382
1	1.848836	0.094075	-0.885382

**(CH<sub>3</sub>, CF<sub>3</sub>, H)**

6	-1.741292	-1.147711	0.000000
1	-1.428574	-1.708181	0.886256
1	-1.428574	-1.708181	-0.886256
1	-2.833765	-1.089835	0.000000
6	-1.136547	0.258329	0.000000
1	-1.454252	0.824186	-0.882254
1	-1.454252	0.824186	0.882254
6	0.375473	0.249524	0.000000
9	0.874578	1.505997	0.000000
9	0.874578	-0.380945	-1.088673
9	0.874578	-0.380945	1.088673

**(CH<sub>3</sub>, CH<sub>3</sub>, H)**

6	0.000000	1.277178	-0.259897
6	0.000000	0.000000	0.586502
6	0.000000	-1.277178	-0.259897
1	0.000000	2.176122	0.367439
1	0.884640	1.322072	-0.907416
1	-0.884640	1.322072	-0.907416
1	0.877624	0.000000	1.247269
1	-0.877624	0.000000	1.247269
1	0.884640	-1.322072	-0.907416
1	-0.884640	-1.322072	-0.907416
1	0.000000	-2.176122	0.367439

**(CH<sub>3</sub>, CH=CH<sub>2</sub>, H)**

6	-1.729367	-0.246447	-0.294650
1	-1.931162	-1.168015	0.264778
1	-1.527816	-0.526509	-1.334504
1	-2.640651	0.361991	-0.275245
6	-0.540175	0.520606	0.308220
1	-0.366282	1.444342	-0.258163
1	-0.800613	0.826003	1.332862
6	0.723419	-0.296157	0.340058
6	1.861747	0.017853	-0.279405
1	0.672374	-1.223455	0.914785
1	2.740836	-0.618845	-0.223479
1	1.959569	0.929358	-0.866370

**(CH<sub>3</sub>, CHO, H)**

6	1.439527	-0.506290	0.000107
1	1.245721	-1.124863	-0.881316
1	1.245496	-1.125103	0.881312
1	2.497479	-0.225440	0.000280

6	0.549040	0.734047	0.000162
1	0.746688	1.376853	0.872389
1	0.746894	1.377078	-0.871853
6	-0.931190	0.425483	-0.000054
8	-1.403919	-0.689829	-0.000261
1	-1.595187	1.320662	-0.000012

**(CH<sub>3</sub>, Cl, H)**

6	-1.512104	0.678948	0.000000
1	-1.858333	0.141174	0.887528
1	-1.858333	0.141174	-0.887528
1	-1.969619	1.676308	0.000000
6	0.000000	0.821192	0.000000
1	0.361587	1.343043	-0.888113
1	0.361587	1.343043	0.888113
17	0.825632	-0.802681	0.000000

**(CH<sub>3</sub>, CN, H)**

6	-1.519856	0.567386	0.000000
1	-1.825677	0.003881	0.886245
1	-1.825677	0.003881	-0.886245
1	-2.048039	1.525826	0.000000
6	0.000000	0.812623	0.000000
1	0.293453	1.398384	-0.879660
1	0.293453	1.398384	0.879660
6	0.773039	-0.434118	0.000000
7	1.370484	-1.429386	0.000000

**(CH<sub>3</sub>, F, H)**

6	-1.124635	-0.457208	0.000000
1	-1.065908	-1.095284	0.887742
1	-1.065908	-1.095284	-0.887742
1	-2.097571	0.047637	0.000000
6	0.000000	0.559700	0.000000
1	-0.041463	1.201055	-0.889691
1	-0.041463	1.201055	0.889691
9	1.228902	-0.097125	0.000000

**(CH<sub>3</sub>, NH<sub>2</sub>, H)**

6	-1.216831	-0.360442	0.000000
1	-1.215350	-1.007975	0.886296
1	-1.215350	-1.007975	-0.886296
1	-2.157833	0.204253	0.000000
6	0.000000	0.574339	0.000000
1	-0.040605	1.232672	-0.877095
1	-0.040605	1.232672	0.877095

7	1.313687	-0.079157	0.000000
1	1.387459	-0.691462	0.812519
1	1.387459	-0.691462	-0.812519

**(CH<sub>3</sub>, OH, H)**

6	-1.172839	-0.410733	0.000000
1	-1.138323	-1.052041	0.886836
1	-1.138323	-1.052041	-0.886836
1	-2.122985	0.134946	0.000000
6	0.000000	0.555587	0.000000
1	-0.051037	1.207894	-0.887529
1	-0.051037	1.207894	0.887529
8	1.198889	-0.214552	0.000000
1	1.947628	0.400634	0.000000

**(CH<sub>3</sub>, SH, H)**

6	-1.521791	0.706526	0.000000
1	-1.874857	0.169948	0.887011
1	-1.874857	0.169948	-0.887011
1	-1.981704	1.701189	0.000000
6	0.000000	0.835922	0.000000
1	0.338552	1.378132	-0.887682
1	0.338552	1.378132	0.887682
16	0.758516	-0.850130	0.000000
1	2.048801	-0.449968	0.000000

**(F, BH<sub>2</sub>, H)**

6	0.000000	0.493389	0.000000
1	0.032815	1.166771	0.875094
1	0.032815	1.166771	-0.875094
5	-1.340418	-0.298149	0.000000
1	-2.355356	0.334814	0.000000
1	-1.375662	-1.490373	0.000000
9	1.151942	-0.294175	0.000000

**(F, CCH, H)**

6	0.667153	-0.526661	0.000000
1	1.302301	-0.631535	0.888913
1	1.302301	-0.631535	-0.888913
9	-0.255600	-1.567118	0.000000
6	0.000000	0.772763	0.000000
6	-0.546419	1.848434	0.000000
1	-1.028606	2.799921	0.000000

**(F, CF<sub>3</sub>, H)**

6	1.156739	0.239929	0.000000
1	1.494024	0.770516	0.895974
1	1.494024	0.770516	-0.895974
9	1.654341	-1.043685	0.000000
6	-0.361443	0.192580	0.000000
9	-0.838848	-0.436361	1.087413
9	-0.838848	-0.436361	-1.087413
9	-0.838848	1.456842	0.000000

**(F, CH=CH<sub>2</sub>, H)**

6	0.945345	-0.205997	0.000000
1	1.595975	-0.177923	0.886709
1	1.595975	-0.177923	-0.886709
9	0.265466	-1.415503	0.000000
6	0.000000	0.957250	0.000000
6	-1.326182	0.844024	0.000000
1	0.479627	1.936297	0.000000
1	-1.971074	1.717544	0.000000
1	-1.804673	-0.130133	0.000000

**(F, CHO, H)**

6	0.000000	0.744708	0.000000
1	-0.464411	1.187522	0.890593
1	-0.464411	1.187522	-0.890593
9	1.357155	1.011957	0.000000
6	-0.226992	-0.758357	0.000000
8	-1.328754	-1.254743	0.000000
1	0.706410	-1.362820	0.000000

**(F, Cl, H)**

6	0.000000	0.816934	0.000000
1	-0.356485	1.310907	0.905470
1	-0.356485	1.310907	-0.905470
9	1.358258	0.776792	0.000000
17	-0.677139	-0.853797	0.000000

**(F, CN, H)**

6	0.637098	-0.514499	0.000000
1	1.266158	-0.616283	0.891892
1	1.266158	-0.616283	-0.891892
9	-0.320137	-1.507834	0.000000
6	0.000000	0.811854	0.000000
7	-0.496239	1.859849	0.000000

**(F, F, H)**



6	0.000000	0.000000	0.499051
1	0.909576	0.000000	1.110123
1	-0.909576	0.000000	1.110123
9	0.000000	1.109050	-0.289697
9	0.000000	-1.109050	-0.289697

**(F, NH<sub>2</sub>, H)**

6	0.000000	0.530826	0.000000
1	0.022112	1.159072	0.895950
1	0.022112	1.159072	-0.895950
9	1.188607	-0.226206	0.000000
7	-1.183188	-0.252602	0.000000
1	-1.229686	-0.849518	-0.822314
1	-1.229686	-0.849518	0.822314

**(F, OH, H)**

6	0.017654	0.508601	0.049341
1	0.068192	1.018866	1.022021
1	0.057101	1.230572	-0.770585
9	1.135128	-0.309655	-0.029137
8	-1.150161	-0.212378	-0.115581
1	-1.246083	-0.815126	0.639396

**(F, SH, H)**

6	-0.589510	0.564022	0.086142
1	-0.711623	1.310422	-0.704704
1	-0.724920	1.033733	1.064118
9	-1.543198	-0.420882	-0.063651
16	1.108097	-0.074350	-0.086576
1	1.132836	-0.750744	1.081816

**(Cl, BH<sub>2</sub>, H)**

6	0.000000	0.831241	0.000000
1	0.425306	1.342650	0.873396
1	0.425306	1.342650	-0.873396
17	0.659073	-0.863802	0.000000
5	-1.553869	0.975490	0.000000
1	-2.296215	0.043619	0.000000
1	-1.989300	2.090821	0.000000

**(Cl, CCH, H)**

6	0.000000	0.833332	0.000000
1	0.107510	1.459789	0.888482
1	0.107510	1.459789	-0.888482
17	1.444327	-0.291341	0.000000

6	-1.261814	0.120342	0.000000
6	-2.323538	-0.453098	0.000000
1	-3.256459	-0.970238	0.000000

**(Cl, CF<sub>3</sub>, H)**

6	0.855094	0.494459	0.000000
1	1.183682	1.027564	0.892631
1	1.183682	1.027564	-0.892631
17	1.608091	-1.132517	0.000000
6	-0.663625	0.426764	0.000000
9	-1.142731	-0.197366	1.087676
9	-1.142731	-0.197366	-1.087676
9	-1.142731	1.691435	0.000000

**(Cl, CH=CH<sub>2</sub>, H)**

6	-0.026710	0.747958	0.124656
1	0.125313	1.305343	-0.801100
1	-0.263973	1.444116	0.932607
17	-1.553541	-0.241845	-0.109346
6	1.141202	-0.120775	0.453521
6	2.232170	-0.205107	-0.308596
1	1.068523	-0.691020	1.377995
1	3.077208	-0.826632	-0.026575
1	2.323162	0.347105	-1.241529

**(Cl, CHO, H)**

6	0.029508	0.661386	0.121826
1	0.173557	1.358646	-0.704804
1	0.002031	1.220543	1.062878
17	-1.565918	-0.159715	-0.067911
6	1.171808	-0.344138	0.163134
8	2.290723	-0.052261	-0.183400
1	0.911345	-1.349420	0.553848

**(Cl, Cl, H)**

6	0.000000	0.000000	0.767813
1	-0.899046	0.000000	1.379813
1	0.899046	0.000000	1.379813
17	0.000000	1.496256	-0.216662
17	0.000000	-1.496256	-0.216662

**(Cl, CN, H)**

6	0.000000	0.819043	0.000000
1	0.090127	1.445049	0.890206
1	0.090127	1.445049	-0.890206

17	1.394419	-0.334224	0.000000
6	-1.282988	0.124686	0.000000
7	-2.312492	-0.410094	0.000000

**(Cl, NH<sub>2</sub>, H)**

6	0.000000	0.855818	0.000000
1	0.419345	1.307453	0.897022
1	0.419345	1.307453	-0.897022
17	0.741613	-0.894147	0.000000
7	-1.401637	0.920742	0.000000
1	-1.817322	0.502748	0.827092
1	-1.817322	0.502748	-0.827092

**(Cl, OH, H)**

6	-0.589401	0.589710	0.043762
1	-0.631712	1.119231	0.999805
1	-0.649571	1.281599	-0.794225
17	1.115956	-0.125075	-0.010141
8	-1.572252	-0.358722	-0.119039
1	-1.575553	-0.943028	0.656561

**(Cl, SH, H)**

6	-0.001623	0.762089	0.074738
1	-0.022306	1.469819	-0.753573
1	-0.041698	1.302000	1.019313
17	-1.531179	-0.217160	-0.023330
16	1.540434	-0.177121	-0.088396
1	1.456849	-0.818686	1.096768

**(NH<sub>2</sub>, BH<sub>2</sub>, H)**

7	0.492664	-0.668404	0.000004
1	0.896941	-1.067327	-0.839712
1	0.896966	-1.067329	0.839708
6	0.282488	0.831579	-0.000004
1	0.682597	1.287328	-0.903749
1	0.682582	1.287342	0.903738
5	-1.025125	-0.049545	-0.000001
1	-1.588523	-0.251487	-1.038805
1	-1.588512	-0.251450	1.038818

**(NH<sub>2</sub>, CCH, H)**

7	-0.099199	-1.670278	0.000000
1	-0.716192	-1.646401	0.811237
1	-0.716192	-1.646401	-0.811237
6	0.733527	-0.457593	0.000000

1	1.392356	-0.500884	-0.876257
1	1.392356	-0.500884	0.876257
6	0.000000	0.819903	0.000000
6	-0.642599	1.843669	0.000000
1	-1.203505	2.750646	0.000000

**(NH<sub>2</sub>, CF<sub>3</sub>, H)**

7	1.770120	-1.082507	0.000000
1	1.461456	-1.606395	0.816899
1	1.461456	-1.606395	-0.816899
6	1.160316	0.236507	0.000000
1	1.489403	0.794218	-0.882861
1	1.489403	0.794218	0.882861
6	-0.361191	0.239994	0.000000
9	-0.855086	-0.395602	1.089012
9	-0.855086	1.495970	0.000000
9	-0.855086	-0.395602	-1.089012

**(NH<sub>2</sub>, CH=CH<sub>2</sub>, H)**

7	1.471256	-0.565762	0.000000
1	1.221661	-1.126018	0.814047
1	1.221661	-1.126017	-0.814048
6	0.700255	0.674756	0.000000
1	1.015068	1.266543	-0.872095
1	1.015068	1.266543	0.872096
6	-0.810673	0.577592	0.000000
6	-1.521077	-0.550201	0.000000
1	-1.333050	1.536227	0.000000
1	-2.607137	-0.542524	0.000000
1	-1.043087	-1.527301	0.000000

**(NH<sub>2</sub>, CHO, H)**

7	1.454455	-0.493480	-0.000003
1	1.212250	-1.067898	0.806694
1	1.212196	-1.067947	-0.806649
6	0.612787	0.690732	-0.000006
1	0.849489	1.318458	-0.872908
1	0.849507	1.318471	0.872882
6	-0.888278	0.447014	0.000006
8	-1.391604	-0.654974	-0.000002
1	-1.518847	1.366589	0.000017

**(NH<sub>2</sub>, CN, H)**

7	1.456774	0.721301	0.000000
1	1.767092	0.197255	0.816017
1	1.767092	0.197255	-0.816017

6	0.000000	0.831028	0.000000
1	-0.313354	1.406176	-0.878336
1	-0.313354	1.406176	0.878336
6	-0.730399	-0.458253	0.000000
7	-1.246071	-1.498946	0.000000

**(NH<sub>2</sub>, NH<sub>2</sub>, H)**

7	0.000000	1.266784	-0.182352
1	0.816214	1.319017	-0.791486
1	-0.816210	1.319013	-0.791492
6	0.000000	0.000000	0.552115
1	-0.880915	0.000003	1.203095
1	0.880915	-0.000003	1.203095
7	0.000000	-1.266784	-0.182352
1	-0.816214	-1.319017	-0.791486
1	0.816210	-1.319013	-0.791492

**(NH<sub>2</sub>, OH, H)**

7	1.222289	-0.209772	0.000000
1	1.245685	-0.819353	0.816044
1	1.245685	-0.819353	-0.816044
6	0.000000	0.537917	0.000000
1	-0.011263	1.182939	-0.891151
1	-0.011263	1.182939	0.891151
8	-1.135729	-0.336908	0.000000
1	-1.939037	0.209000	0.000000

**(NH<sub>2</sub>, SH, H)**

7	1.668299	-0.276222	0.000002
1	1.650016	-0.876182	0.821493
1	1.650021	-0.876204	-0.821473
6	0.567550	0.644414	-0.000004
1	0.620537	1.275726	-0.889416
1	0.620528	1.275736	0.889402
16	-1.108220	-0.225556	-0.000001
1	-1.892982	0.876883	0.000025

**(OH, BH<sub>2</sub>, H)**

6	0.021695	-0.499886	0.027410
1	0.079319	-1.093474	0.969140
5	1.357872	0.292615	-0.030030
1	1.384584	1.491288	0.008117
1	2.389250	-0.312167	-0.056830
8	-1.215530	0.202173	-0.053890
1	-1.059651	1.107504	0.252513
1	0.011207	-1.274298	-0.756130

**(OH, CCH, H)**

6	-0.627969	0.587239	0.036643
1	-0.841756	1.267545	-0.794813
1	-0.805875	1.151887	0.966518
8	-1.549597	-0.488558	-0.102226
1	-1.326932	-1.148352	0.573305
6	0.776884	0.161771	-0.008279
6	1.923384	-0.218167	-0.010853
1	2.937545	-0.547676	-0.032266

**(OH, CF<sub>3</sub>, H)**

6	0.895129	0.772921	-0.084587
1	0.916587	1.526940	0.705839
1	0.909905	1.287383	-1.056680
8	2.003548	-0.072655	0.109528
1	1.984930	-0.746062	-0.589427
6	-0.420348	0.015204	0.007763
9	-0.443460	-0.991236	-0.903505
9	-0.617312	-0.533143	1.217656
9	-1.460171	0.833738	-0.255819

**(OH, CH=CH<sub>2</sub>, H)**

6	-0.734710	0.632358	0.041143
1	-1.127983	1.265102	-0.774330
1	-1.042624	1.116823	0.977120
8	-1.355767	-0.642001	0.049310
1	-1.106585	-1.084785	-0.777628
6	0.770085	0.592827	-0.044719
6	1.504668	-0.515974	0.038167
1	1.252426	1.560149	-0.191220
1	2.587651	-0.490720	-0.038736
1	1.042995	-1.485821	0.202764

**(OH, CHO, H)**

6	-0.676624	0.648543	0.000006
1	-0.954692	1.252577	-0.882122
1	-0.954667	1.252558	0.882159
8	-1.326545	-0.590053	-0.000008
1	-0.614002	-1.258175	0.000027
6	0.826801	0.493994	-0.000008
8	1.350977	-0.601019	0.000003
1	1.426841	1.426395	-0.000014

**(OH, CN, H)**

6	-0.573447	0.591008	0.038325
1	-0.742334	1.279920	-0.794571
1	-0.717002	1.158033	0.970466
8	-1.509253	-0.456799	-0.112258
1	-1.403391	-1.068482	0.633735
6	0.827729	0.120212	-0.006579
7	1.915865	-0.283200	-0.014578

**(OH, OH, H)**

6	0.000000	0.531273	0.000000
1	0.011593	1.165082	0.895845
1	-0.011597	1.165082	-0.895845
8	1.169648	-0.245762	0.090708
1	1.208140	-0.792806	-0.711144
8	-1.169648	-0.245762	-0.090708
1	-1.208136	-0.792807	0.711144

**(OH, SH, H)**

6	0.588066	0.596243	0.040713
1	0.658127	1.284373	-0.812825
1	0.694095	1.169144	0.963108
8	1.597905	-0.373332	0.055341
1	1.508422	-0.907011	-0.751051
16	-1.130532	-0.085045	-0.073259
1	-1.083779	-0.776586	1.085907

**(SH, BH<sub>2</sub>, H)**

6	0.758192	0.809382	0.026908
1	0.841384	1.423210	-0.869958
5	1.243875	-0.669783	0.007069
1	1.418401	-1.250096	1.037418
1	1.525544	-1.179134	-1.036041
1	0.777653	1.418187	0.929989
16	-0.888581	-0.106233	-0.093143
1	-1.114210	-0.219821	1.232085

**(SH, CCH, H)**

6	-0.004249	0.842206	0.063032
1	-0.118339	1.540484	-0.773164
1	-0.089340	1.425207	0.985472
16	-1.476027	-0.282016	-0.078489
1	-1.149019	-1.076719	0.962900
6	1.277929	0.158917	-0.002826
6	2.342035	-0.410796	-0.034283
1	3.278831	-0.918681	-0.074927

**(SH, CF<sub>3</sub>, H)**

6	0.434485	0.848535	-0.237919
1	0.407016	1.699260	0.446882
1	0.392199	1.232179	-1.259946
16	2.016987	-0.014185	0.076108
1	1.885378	-0.922863	-0.913346
6	-0.804331	0.004922	0.005316
9	-0.833026	-1.076663	-0.803923
9	-0.893668	-0.427237	1.273826
9	-1.910785	0.736971	-0.258313

**(SH, CH=CH<sub>2</sub>, H)**

6	0.021742	0.763841	-0.109051
1	0.248608	1.676152	0.454398
1	-0.157354	1.049141	-1.149575
16	1.594311	-0.213148	0.003596
1	1.142920	-1.296566	-0.664688
6	-1.156111	0.045354	0.472272
6	-2.240485	-0.296648	-0.225884
1	-1.082404	-0.211659	1.528243
1	-3.073944	-0.819972	0.234228
1	-2.337678	-0.062003	-1.284162

**(SH, CHO, H)**

6	0.022396	0.781938	-0.165211
1	0.205107	1.029321	-1.212965
1	-0.152901	1.700920	0.405174
16	-1.525087	-0.199854	0.037948
1	-1.158330	-1.218752	-0.769664
6	1.198289	0.022001	0.411824
8	2.131985	-0.369000	-0.251276
1	1.1 <sub>2</sub> 75 <sub>3</sub> 5	-0.18546 <sub>2</sub>	1.50081 <sub>2</sub>

**(SH, CN, H)**

6	0.048194	0.825862	0.065495
1	-0.018285	1.527902	-0.771145
1	0.008093	1.408115	0.990498
16	-1.445026	-0.251557	-0.082116
1	-1.201271	-0.987452	1.023335
6	1.310815	0.095178	-0.005572
7	2.311118	-0.492843	-0.041197

**(SH, SH, H)**

6	0.000002	0.777592	-0.000005
1	0.024351	1.420610	0.882288



1	-0.024340	1.420616	-0.882293
16	1.564151	-0.179653	0.057732
1	1.358981	-0.878965	-1.078940
16	-1.564151	-0.179654	-0.057732
1	-1.359006	-0.878903	1.078982

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, H)**

1	0.836143	-0.758171	-1.397982
6	0.899476	-0.615359	-0.317187
1	1.494836	-1.403648	0.146582
6	-0.455168	-0.490141	0.338051
6	-1.467711	0.242516	-0.160492
1	-0.551905	-0.897172	1.343217
1	-2.392178	0.384492	0.392336
1	-1.415336	0.690018	-1.149605
5	1.147873	0.860813	0.161606
1	0.975937	1.766646	-0.599381
1	1.453559	1.091679	1.294566

**(CH=CH<sub>2</sub>, CCH, H)**

6	0.000000	1.036354	0.000000
1	-0.052954	1.705420	0.872955
1	-0.052954	1.705420	-0.872955
6	-1.165532	0.152060	0.000000
6	-2.128056	-0.576719	0.000000
1	-2.982812	-1.214118	0.000000
6	1.346507	0.339473	0.000000
6	1.549778	-0.975896	0.000000
1	2.196932	1.021100	0.000000
1	2.553931	-1.390188	0.000000
1	0.721679	-1.679266	0.000000

**(CH=CH<sub>2</sub>, CF<sub>3</sub>, H)**

1	0.604410	-1.448205	-0.673298
6	0.453951	-0.366246	-0.742147
6	-0.819140	-0.028818	0.011155
1	0.260176	-0.123673	-1.795161
6	1.656089	0.383372	-0.233937
6	2.784443	-0.196809	0.170907
1	1.568221	1.468708	-0.221454
1	3.633344	0.388202	0.513150
1	2.905728	-1.278031	0.173795
9	-0.737206	-0.352491	1.317853
9	-1.877972	-0.691952	-0.505429
9	-1.098593	1.293777	-0.060524

**(CH=CH<sub>2</sub>, CH=CH<sub>2</sub>, H)**

6	0.000000	0.000000	0.664349
1	-0.804959	0.364706	1.318325
1	0.804959	-0.364706	1.318325
6	0.506065	1.147240	-0.178189
6	0.000000	2.380662	-0.176212
1	1.340622	0.910621	-0.839324
1	0.403047	3.166140	-0.810021
1	-0.836337	2.654673	0.464377
6	-0.506065	-1.147240	-0.178189
6	0.000000	-2.380662	-0.176212
1	-1.340622	-0.910621	-0.839324
1	-0.403047	-3.166140	-0.810021
1	0.836337	-2.654673	0.464377

**(CH=CH<sub>2</sub>, CHO, H)**

1	0.209258	1.126265	-1.087788
6	-0.057878	0.703910	-0.108744
1	-0.425300	1.510249	0.535602
6	1.141598	0.010468	0.489014
6	2.273046	-0.254251	-0.165331
1	1.032579	-0.311607	1.524544
1	3.098063	-0.776103	0.311650
1	2.423179	0.050121	-1.199303
6	-1.201162	-0.280199	-0.323552
8	-2.289617	-0.194335	0.196731
1	-0.954471	-1.123811	-1.006875

**(CH=CH<sub>2</sub>, CN, H)**

1	0.056485	1.690942	0.876092
6	0.000000	1.029223	0.000000
1	0.056485	1.690942	-0.876092
6	-1.318702	0.282323	0.000000
6	-1.469228	-1.039873	0.000000
1	-2.190996	0.934147	0.000000
1	-2.457688	-1.489428	0.000000
1	-0.619223	-1.717243	0.000000
6	1.182927	0.163522	0.000000
7	2.112137	-0.531504	0.000000

**(CCH, BH<sub>2</sub>, H)**

6	0.844146	-0.704935	0.000034
1	1.108873	-1.271593	0.897687
1	1.109054	-1.271686	-0.897508
5	1.218386	0.831135	0.000043
1	1.329697	1.411298	-1.036976
1	1.330492	1.411124	1.037078

6	-0.570383	-0.333274	-0.000049
6	-1.660151	0.200236	-0.000057
1	-2.651717	0.593017	-0.000062

**(CCH, CCH, H)**

6	0.000000	0.000000	0.876774
1	0.876405	0.000000	1.541395
1	-0.876405	0.000000	1.541395
6	0.000000	1.229680	0.072474
6	0.000000	2.247072	-0.574996
1	0.000000	3.140819	-1.156582
6	0.000000	-1.229680	0.072474
6	0.000000	-2.247072	-0.574996
1	0.000000	-3.140819	-1.156582

**(CCH, CF<sub>3</sub>, H)**

6	-0.939637	0.476881	0.000000
6	0.584273	0.440743	0.000000
1	-1.247498	1.050361	0.882330
1	-1.247498	1.050361	-0.882330
6	-1.553331	-0.847243	0.000000
6	-2.071870	-1.935642	0.000000
1	-2.520424	-2.903270	0.000000
9	1.070326	1.702102	0.000000
9	1.070326	-0.184711	1.088111
9	1.070326	-0.184711	-1.088111

**(CCH, CHO, H)**

6	0.021885	0.719827	0.086371
1	0.269255	1.362030	-0.766853
1	0.099124	1.350035	0.987196
6	-1.320901	0.156858	-0.017026
6	-2.412403	-0.351675	-0.100772
1	-3.381754	-0.789395	-0.179297
6	1.109905	-0.353493	0.204923
8	2.227416	-0.209493	-0.228034
1	0.803131	-1.275828	0.742256

**(CCH, CN, H)**

6	0.000000	0.863053	0.000000
1	0.000473	1.521758	0.879267
1	0.000473	1.521758	-0.879267
6	1.193343	0.011837	0.000000
6	2.181914	-0.677223	0.000000
1	3.051811	-1.294665	0.000000
6	-1.256477	0.094239	0.000000

7	-2.252205	-0.500041	0.000000
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**(CF<sub>3</sub>, BH<sub>2</sub>, H)**

6	0.934093	0.765748	-0.000003
6	-0.377492	0.021975	0.000000
1	0.956598	1.437542	-0.870578
1	0.956597	1.437553	0.870564
9	-0.496330	-0.771283	1.089828
9	-1.440903	0.859598	-0.000001
9	-0.496332	-0.771288	-1.089824
5	2.232584	-0.116560	0.000001
1	2.194611	-1.308528	-0.000004
1	3.291760	0.436660	0.000006

**(CF<sub>3</sub>, CF<sub>3</sub>, H)**

6	0.000000	1.279805	0.074908
6	0.000000	0.000000	0.892860
6	0.000000	-1.279805	0.074908
1	-0.886524	0.000000	1.531341
1	0.886524	0.000000	1.531341
9	0.000000	2.344253	0.905787
9	1.087965	1.373238	-0.711747
9	-1.087965	1.373238	-0.711747
9	1.087965	-1.373238	-0.711747
9	0.000000	-2.344253	0.905787
9	-1.087965	-1.373238	-0.711747

**(CF<sub>3</sub>, CHO, H)**

6	0.806264	-0.029813	0.007242
6	-0.502072	-0.639745	-0.448280
1	-0.427808	-0.811768	-1.529993
1	-0.657539	-1.601895	0.045358
6	-1.697482	0.266653	-0.183456
8	-2.770661	-0.150603	0.180739
1	-1.528101	1.346490	-0.373823
9	0.792486	0.223510	1.332982
9	1.042063	1.143580	-0.624701
9	1.847504	-0.846043	-0.246114

**(CF<sub>3</sub>, CN, H)**

6	0.574815	0.421884	0.000000
6	-0.951792	0.458464	0.000000
1	-1.278266	1.013280	0.885582
1	-1.278266	1.013280	-0.885582
6	-1.550557	-0.875854	0.000000
7	-2.035442	-1.928862	0.000000

9	1.050734	-0.205298	1.088292
9	1.050734	1.682653	0.000000
9	1.050734	-0.205298	-1.088292

**(BH<sub>2</sub>, BH<sub>2</sub>, H)**

6	0.000000	0.559038	0.184476
1	-0.000001	1.535141	-0.307434
1	0.000000	0.664267	1.285174
5	1.271158	-0.298355	-0.115274
1	1.515592	-1.261832	0.551448
1	2.008042	-0.023209	-1.017377
5	-1.271157	-0.298356	-0.115274
1	-1.515593	-1.261832	0.551447
1	-2.008041	-0.023208	-1.017377

**(BH<sub>2</sub>, CHO, H)**

6	0.579878	-0.517745	0.226672
1	0.878382	-0.725607	1.276413
1	0.429493	-1.482265	-0.268002
5	1.827235	0.294143	-0.265621
1	1.883634	1.477899	-0.099869
1	2.759708	-0.270713	-0.753316
6	-0.705408	0.269288	0.271652
8	-1.708539	-0.020467	-0.340345
1	-0.665898	1.184451	0.905693

**(BH<sub>2</sub>, CN, H)**

6	-0.642998	-0.511114	0.000000
1	-1.317423	-0.593209	0.867728
1	-1.317423	-0.593209	-0.867728
5	0.304479	-1.773077	0.000000
1	1.492198	-1.679507	0.000000
1	-0.215423	-2.848333	0.000000
6	0.000000	0.800562	0.000000
7	0.527666	1.834708	0.000000

**(CHO, CHO, H)**

6	0.023807	0.765729	0.262552
1	-0.074277	0.962680	1.342064
1	0.396970	1.675871	-0.214895
6	-1.351931	0.360330	-0.240293
8	-1.868758	-0.697506	0.043604
1	-1.866265	1.091953	-0.898956
6	1.044487	-0.358991	0.110830
8	2.193208	-0.172638	-0.212855
1	0.649790	-1.371760	0.327259

**(CHO, CN, H)**

6	-0.027909	0.690714	0.094325
1	0.183515	1.362929	-0.743764
1	0.024140	1.292542	1.013607
6	1.084968	-0.367910	0.171410
8	2.209138	-0.140870	-0.197788
1	0.790618	-1.341279	0.613407
6	-1.363017	0.107293	-0.020932
7	-2.405090	-0.395403	-0.109966

**(CN, CN, H)**

6	0.000000	0.000000	0.840191
1	-0.882412	0.000000	1.492704
1	0.882412	0.000000	1.492704
6	0.000000	1.224136	0.026633
7	0.000000	2.201560	-0.596153
6	0.000000	-1.224136	0.026633
7	0.000000	-2.201560	-0.596153

**(COOH, BH<sub>2</sub>, H)**

6	0.893840	-0.275244	0.554703
1	1.062926	-1.295653	0.915918
1	1.061871	0.393841	1.416477
6	-0.525356	-0.141530	0.078027
8	-1.232833	-1.045959	-0.306894
8	-0.938699	1.153749	0.087589
1	-1.844195	1.147559	-0.275652
5	2.000157	0.150371	-0.478204
1	1.740390	0.758934	-1.472114
1	3.139573	-0.118205	-0.235553

**(COOH, CCH, H)**

6	0.258992	-0.859704	0.353333
1	0.146977	-1.831795	-0.137219
1	0.208259	-1.047820	1.436310
6	-0.984760	-0.047965	-0.003075
8	-2.021086	-0.535381	-0.390157
8	-0.820420	1.273674	0.215009
1	-1.671904	1.692869	-0.012993
6	1.537453	-0.239367	0.016670
6	2.606084	0.245486	-0.262049
1	3.542102	0.689707	-0.514184

**(COOH, CF<sub>3</sub>, H)**

6	0.171819	-0.572874	-0.744353
1	0.124968	-1.662510	-0.739730
1	0.105032	-0.218400	-1.778069
6	1.508994	-0.163021	-0.150881
8	2.371562	-0.936824	0.189625
8	1.636972	1.179384	-0.073346
1	2.515004	1.348977	0.318497
6	-1.036852	-0.038251	0.006233
9	-0.951602	-0.309463	1.326037
9	-2.162012	-0.621749	-0.461023
9	-1.183834	1.290803	-0.131339

**(COOH, CH<sub>3</sub>, H)**

6	0.771168	-0.511734	0.502576
1	0.833001	-1.601869	0.459969
1	0.889791	-0.206815	1.550188
6	-0.626323	-0.131262	0.063854
8	-1.491769	-0.895189	-0.301513
8	-0.824334	1.212899	0.122337
1	-1.740028	1.360677	-0.180417
6	1.870554	0.142274	-0.350332
1	2.858113	-0.175412	-0.000559
1	1.818009	1.232867	-0.289576
1	1.777541	-0.146798	-1.402772

**(COOH, CH=CH<sub>2</sub>, H)**

6	0.291703	-0.343151	0.747599
1	0.493935	-1.416130	0.777121
1	0.154792	0.008337	1.781109
6	-1.036952	-0.152112	0.035711
8	-1.750041	-1.035440	-0.380587
8	-1.358938	1.162645	-0.077631
1	-2.214294	1.190543	-0.546474
6	1.426226	0.413586	0.100867
6	2.512844	-0.164109	-0.409939
1	1.314787	1.495682	0.064230
1	3.308900	0.421846	-0.860954
1	2.650791	-1.243204	-0.394712

**(COOH, CHO, H)**

6	-0.325534	-0.532292	0.454158
1	-0.354339	-0.552758	1.554721
1	-0.424282	-1.562146	0.104662
6	0.997043	0.086615	0.056904
8	1.219786	1.276751	0.021762
8	1.921043	-0.849972	-0.251609
1	2.737711	-0.365054	-0.479599

6	-1.515437	0.301761	-0.008025
8	-2.586223	-0.183054	-0.288419
1	-1.332368	1.393647	-0.051884

**(COOH, Cl, H)**

6	0.298039	-0.662886	0.556615
1	0.323850	-1.729636	0.342922
1	0.377482	-0.490573	1.632709
6	-1.016184	-0.102017	0.041704
8	-1.908963	-0.788922	-0.397420
8	-1.093441	1.235990	0.177073
1	-1.966842	1.498464	-0.170205
17	1.740800	0.102036	-0.213680

**(COOH, CN, H)**

6	0.292391	-0.877440	0.261451
1	0.211913	-1.789962	-0.336298
1	0.266586	-1.184413	1.315749
6	-0.965071	-0.046748	0.000301
8	-2.033363	-0.536620	-0.273036
8	-0.750681	1.271531	0.160954
1	-1.604523	1.717292	0.000787
6	1.562010	-0.203706	-0.009513
7	2.580342	0.306452	-0.228146

**(COOH, F, H)**

6	-0.788905	-0.708756	0.000013
1	-0.875607	-1.345508	0.888537
1	-0.875611	-1.345563	-0.888468
6	0.599767	-0.092215	-0.000002
8	1.605119	-0.765839	-0.000009
8	0.584034	1.251959	0.000006
1	1.519288	1.532626	0.000008
9	-1.794052	0.230590	-0.000013

**(COOH, NH<sub>2</sub>, H)**

6	-0.727944	-0.738219	0.000024
1	-0.692775	-1.400450	0.874017
1	-0.692759	-1.400517	-0.873917
6	0.541070	0.108054	0.000003
8	0.573606	1.318701	0.000008
8	1.657306	-0.660653	-0.000016
1	2.414662	-0.044972	-0.000010
7	-1.970276	0.013230	-0.000011
1	-1.981610	0.635023	0.807352
1	-1.981636	0.634909	-0.807460



**(COOH, OH, H)**

6	0.744717	-0.750975	0.000005
1	0.718889	-1.407118	-0.883371
1	0.718891	-1.407101	0.883393
6	-0.514512	0.094037	0.000000
8	-0.498967	1.307549	0.000002
8	-1.640787	-0.642224	-0.000003
1	-2.388690	-0.014993	-0.000003
8	1.889870	0.058627	-0.000006
1	1.568754	0.979220	0.000003

**(COOH, SH, H)**

6	-0.247399	-0.775776	0.310041
1	-0.239863	-1.039070	1.374383
1	-0.159248	-1.704336	-0.257298
6	0.958041	0.108750	0.046466
8	0.974818	1.316855	0.094577
8	2.058399	-0.638052	-0.201815
1	2.797757	-0.009770	-0.311668
16	-1.838598	0.005934	-0.150079
1	-1.510667	1.229958	0.314704

**(COOH, COOH, H)**

6	-0.024544	-0.808420	0.277215
1	0.014438	-1.747513	-0.278210
1	-0.024757	-1.084848	1.341407
6	1.222510	0.005520	0.029135
8	1.277427	1.225391	0.024730
8	2.304885	-0.761249	-0.162799
1	3.064062	-0.158879	-0.288349
6	-1.377458	-0.128241	-0.010787
8	-2.368177	-0.796705	-0.171228
8	-1.401056	1.210222	-0.017440
1	-0.481423	1.556810	0.065670

**(BH<sub>2</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	-0.040698	0.752586	0.000000
1	0.779908	1.488999	0.000000
5	-1.356053	1.636843	0.000000
1	-1.828246	1.992174	1.031712
1	-1.828246	1.992174	-1.031712
6	0.117258	-0.067149	1.276984
9	0.117258	0.748284	2.352562
9	-0.906082	-0.937190	1.419284
9	1.260709	-0.775943	1.315273

6	0.117258	-0.067149	-1.276984
9	0.117258	0.748284	-2.352562
9	1.260709	-0.775943	-1.315273
9	-0.906082	-0.937190	-1.419284

**(BH<sub>2</sub>, BH<sub>2</sub>, CF<sub>3</sub>)**

6	0.557954	0.814392	0.000000
1	1.659398	0.711727	0.000000
5	0.274551	1.683657	1.274196
1	-0.572844	1.376532	2.054278
1	0.912630	2.676523	1.448844
5	0.274551	1.683657	-1.274196
1	0.912630	2.676523	-1.448844
1	-0.572844	1.376532	-2.054278
6	-0.082607	-0.552594	0.000000
9	0.274551	-1.278469	1.087705
9	-1.430941	-0.468083	0.000000
9	0.274551	-1.278469	-1.087705

**(BH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000000	0.000000	0.533126
1	0.000000	0.000000	1.622516
5	0.000000	1.392999	-0.159060
1	0.000000	1.517123	-1.345019
1	0.000000	2.368530	0.533229
5	-1.206373	-0.696500	-0.159060
1	-1.313867	-0.758562	-1.345019
1	-2.051207	-1.184265	0.533229
5	1.206373	-0.696500	-0.159060
1	2.051207	-1.184265	0.533229
1	1.313867	-0.758562	-1.345019

**(CF<sub>3</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	0.000073	-0.000510	-0.508943
1	0.000108	-0.000229	-1.601934
6	-1.304307	-0.685008	-0.059191
9	-1.251233	-2.009460	-0.283987
9	-1.540145	-0.491919	1.247883
9	-2.348194	-0.198505	-0.752233
6	0.058830	1.471423	-0.059176
9	1.003076	2.132587	-0.750541
9	-1.114856	2.086671	-0.286645
9	0.341657	1.579870	1.248298
6	1.245565	-0.786863	-0.059064
9	2.365502	-0.079278	-0.289350
9	1.199051	-1.082146	1.249311
9	1.345022	-1.937156	-0.747159

**(NH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.287586	-0.303358	0.540654
1	0.154186	-0.510898	1.595973
7	-0.961034	-0.528003	-0.251040
1	-1.736795	-0.949543	0.249102
1	-0.819857	-0.945649	-1.166798
5	1.562221	-0.058240	-0.191508
1	1.612527	-0.156494	-1.386034
1	2.531346	0.281207	0.421591
5	-0.599392	0.995872	-0.010878
1	-0.277855	1.576249	-1.003112
1	-1.275974	1.533137	0.814566

**(NH<sub>2</sub>, CF<sub>3</sub>, BH<sub>2</sub>)**

6	-0.693475	-0.136055	-0.636037
1	-0.658320	0.036924	-1.709184
7	-1.696763	0.750538	0.045920
1	-1.369808	1.187362	0.902828
1	-2.205959	1.395514	-0.549172
6	0.673800	-0.039030	-0.034188
9	1.328106	1.092124	-0.416193
9	1.438871	-1.080009	-0.403227
9	0.624029	-0.005281	1.321159
5	-1.930439	-0.868980	0.025547
1	-2.824057	-1.191176	-0.699973
1	-1.813330	-1.348497	1.112028

**(NH<sub>2</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	-0.002688	0.546293	-0.521114
1	0.002640	0.477814	-1.613658
7	-0.058705	1.940944	-0.130473
1	-0.007068	2.022056	0.882999
1	0.730841	2.445853	-0.523468
6	-1.286857	-0.146219	-0.047464
9	-1.258290	-1.469870	-0.293434
9	-2.355536	0.365972	-0.675616
9	-1.464021	0.023518	1.280263
6	1.268811	-0.172839	-0.037396
9	2.351317	0.529460	-0.448463
9	1.386436	-1.418141	-0.526590
9	1.318862	-0.241577	1.308649

**(NH<sub>2</sub>, NH<sub>2</sub>, BH<sub>2</sub>)**

6	-0.229634	0.080050	0.498314
1	-0.269631	-0.214202	1.548556

7	0.873660	-0.744904	-0.199385
1	1.415729	-1.389935	0.366903
1	0.541667	-1.154140	-1.067484
7	-1.465740	0.008307	-0.211556
1	-2.208435	-0.461357	0.296709
1	-1.784700	0.925598	-0.502508
5	1.010607	0.869075	-0.064875
1	0.892561	1.426809	-1.120990
1	1.882135	1.197740	0.689890

**(NH<sub>2</sub>, NH<sub>2</sub>, CF<sub>3</sub>)**

6	0.842421	0.004946	-0.448376
1	0.808974	-0.022040	-1.551932
7	1.574859	-1.166390	-0.008695
1	1.524634	-1.223339	1.007898
1	1.158070	-2.011784	-0.392636
7	1.491421	1.172717	0.120146
1	2.468748	1.164135	-0.161513
1	1.064775	2.028552	-0.226572
6	-0.628004	0.005486	-0.005224
9	-1.285762	-1.028658	-0.582367
9	-1.256387	1.145346	-0.381200
9	-0.766259	-0.121400	1.326478

**(NH<sub>2</sub>, NH<sub>2</sub>, NH<sub>2</sub>)**

6	-0.000952	-0.008808	0.359226
1	-0.006716	-0.069138	1.461989
7	0.117473	1.337491	-0.174227
1	-0.663117	1.900839	0.153565
1	0.984038	1.756288	0.154143
7	1.203225	-0.719107	-0.071622
1	1.171511	-1.687679	0.242326
1	1.231833	-0.724512	-1.091744
7	-1.309954	-0.498882	-0.072435
1	-1.337905	-0.502617	-1.092517
1	-1.449150	-1.456844	0.244867

**CN-BH<sub>2</sub>-CH<sub>3</sub>**

6	0.438382	0.113688	-0.436545
1	0.520729	0.136180	-1.531360
5	0.518051	1.580506	0.173429
1	0.877697	1.728080	1.302269
1	0.172017	2.517750	-0.477828
6	1.411897	-0.927389	0.157051
1	1.221199	-1.927658	-0.244274
1	1.322289	-0.968090	1.246522
1	2.442148	-0.650810	-0.089373

6	-0.960956	-0.197229	-0.116911
7	-2.068896	-0.381772	0.186475

**(CN, CN, CN)**

6	0.000000	0.000000	0.508419
1	0.000000	0.000000	1.609708
6	0.000000	1.408746	0.059491
7	0.000000	2.518461	-0.272907
6	-1.220010	-0.704373	0.059491
7	-2.181052	-1.259231	-0.272907
6	1.220010	-0.704373	0.059491
7	2.181052	-1.259231	-0.272907

**(F, BH<sub>2</sub>-BH<sub>2</sub>)**

6	-0.012494	0.000049	0.284951
1	-0.118474	0.000482	1.394524
9	1.350930	-0.005175	-0.042119
5	-0.765350	1.290903	-0.148871
1	-1.886756	1.454221	0.224697
1	-0.230612	2.099593	-0.843138
5	-0.775243	-1.285004	-0.148819
1	-0.246738	-2.097817	-0.843041
1	-1.897870	-1.439684	0.224770

**(F, BH<sub>2</sub>, CN)**

6	0.459249	-0.015749	0.381888
1	0.577749	-0.067298	1.476758
5	1.075098	1.338921	-0.154297
1	1.899215	1.322999	-1.011782
1	0.688325	2.354873	0.331584
9	1.042730	-1.153917	-0.170451
6	-0.982737	-0.007519	0.083314
7	-2.112061	0.031383	-0.183176

**(F, BH<sub>2</sub>, F)**

6	-0.013841	0.000002	0.313865
1	0.018329	0.000094	1.428576
9	0.676769	-1.115849	-0.134399
5	-1.570694	-0.000027	-0.094361
1	-2.131707	1.009579	-0.210102
1	-2.131688	-1.009605	-0.210335
9	0.676741	1.115854	-0.134437

**(F, F, F)**

6	0.000000	0.000000	0.338659
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1	0.000000	0.000000	1.431418
9	0.000000	1.258172	-0.128273
9	-1.089609	-0.629086	-0.128273
9	1.089609	-0.629086	-0.128273

**(NH<sub>2</sub>, BH<sub>2</sub>, CH<sub>3</sub>)**

6	0.177990	-0.136139	0.502124
1	0.195097	0.047851	1.577167
5	-1.070850	-0.854899	-0.138106
1	-0.960361	-1.316437	-1.240694
1	-1.983487	-1.191751	0.562834
7	-0.860087	0.771363	-0.141440
1	-1.387083	1.377402	0.477718
1	-0.563833	1.253650	-0.983724
6	1.546752	-0.053278	-0.136680
1	2.061934	0.898336	0.060329
1	1.486328	-0.198866	-1.222056
1	2.177819	-0.858728	0.256371

**(NH<sub>2</sub>, BH<sub>2</sub>, CN)**

6	-0.217765	-0.119181	0.583853
1	-0.331286	0.043869	1.653048
5	-1.385721	-0.844903	-0.239836
1	-1.115807	-1.323825	-1.298129
1	-2.350052	-1.180738	0.379548
6	1.148875	-0.060685	0.136522
7	2.249216	-0.022318	-0.238994
7	-1.160418	0.758208	-0.215704
1	-1.743956	1.381120	0.334585
1	-0.738539	1.232059	-1.009242

**(NH<sub>2</sub>, BH<sub>2</sub>, F)**

6	-0.244328	-0.160153	0.478510
1	-0.401692	0.043989	1.537629
9	-1.440992	-0.077468	-0.192545
7	0.754158	0.798984	-0.126785
1	0.412731	1.236379	-0.977185
1	1.214947	1.457670	0.493614
5	1.016137	-0.845595	-0.133814
1	1.900140	-1.161435	0.607708
1	0.948976	-1.283387	-1.243360

**(NH<sub>2</sub>, F, CH<sub>3</sub>)**

6	-0.044521	0.012564	0.364463
1	-0.100232	0.118170	1.453726
6	1.334896	-0.439943	-0.077308

1	2.088002	0.289153	0.233955
1	1.371877	-0.522906	-1.170018
1	1.575679	-1.414344	0.356789
9	-0.244047	1.319905	-0.154274
7	-1.062492	-0.892294	-0.052508
1	-1.980784	-0.553454	0.225503
1	-1.062923	-0.985437	-1.066859

**(NH<sub>2</sub>, F, CN)**

6	0.414288	0.032321	0.375805
1	0.572100	0.132517	1.454408
9	0.854193	1.237762	-0.203054
7	1.087639	-1.119880	-0.092020
1	0.980826	-1.243280	-1.095499
1	2.075736	-1.092717	0.143367
6	-1.035187	-0.067784	0.095619
7	-2.172068	-0.126348	-0.122741

**(CCH, CCH, CCH)**

6	0.000000	0.000000	0.525197
1	0.000000	0.000000	1.628327
6	0.000000	1.410642	0.084314
6	0.000000	2.567088	-0.255045
1	0.000000	3.586370	-0.568783
6	1.221652	-0.705321	0.084314
6	2.223163	-1.283544	-0.255045
1	3.105888	-1.793185	-0.568783
6	-1.221652	-0.705321	0.084314
6	-2.223163	-1.283544	-0.255045
1	-3.105888	-1.793185	-0.568783

**(CCH, CCH, CN)**

6	0.439443	0.284114	0.000000
1	1.366915	0.880038	0.000000
6	-0.679678	1.259173	0.000000
7	-1.543328	2.032555	0.000000
6	0.419214	-0.534381	1.226449
6	0.419214	-1.197984	2.231629
1	0.408323	-1.789629	3.119397
6	0.419214	-0.534381	-1.226449
6	0.419214	-1.197984	-2.231629
1	0.408323	-1.789629	-3.119397

**(CH<sub>3</sub>, CH<sub>3</sub>, CH<sub>3</sub>)**

6	0.000000	1.462098	-0.095849
6	0.000000	0.000000	0.372699

1	0.000000	0.000000	1.473255
1	-0.886218	1.997550	0.265480
1	0.886218	1.997550	0.265480
1	0.000000	1.521181	-1.192347
6	1.266214	-0.731049	-0.095849
6	-1.266214	-0.731049	-0.095849
1	1.286820	-1.766263	0.265480
1	1.317382	-0.760591	-1.192347
1	2.173039	-0.231288	0.265480
1	-1.317382	-0.760591	-1.192347
1	-1.286820	-1.766263	0.265480
1	-2.173039	-0.231288	0.265480

**(CHO, CCH, CN)**

6	-0.020771	0.031876	-0.430364
1	-0.252698	-0.159101	-1.485920
6	-0.917145	-0.936539	0.404000
8	-1.643497	-1.743148	-0.110368
1	-0.806000	-0.826047	1.499754
6	-0.378630	1.422101	-0.102421
7	-0.696028	2.500698	0.184062
6	1.385580	-0.259424	-0.139518
6	2.521674	-0.554275	0.136933
1	3.534620	-0.796987	0.368896

**(CHO, CHO, CHO)**

6	-0.020635	-0.000001	0.474332
1	-0.507922	0.000004	1.451358
6	-0.472671	1.249120	-0.310199
8	-1.395695	1.940615	0.036107
1	0.127270	1.457138	-1.217956
6	-0.472690	-1.249116	-0.310194
8	-1.395736	-1.940586	0.036108
1	0.127253	-1.457157	-1.217944
6	1.496474	-0.000010	0.551022
8	2.182687	-0.000021	-0.448645
1	1.940479	-0.000007	1.566225

**(CHO, CHO, CN)**

6	0.067272	-0.153877	0.441967
1	0.274867	-0.206629	1.521563
6	1.300707	-0.763678	-0.259268
8	2.409131	-0.342142	-0.040423
1	1.097386	-1.577993	-0.980976
6	0.002747	1.360397	0.104339
8	-0.991107	1.925568	-0.262372
1	0.978350	1.864481	0.241791



6	-1.171303	-0.861982	0.137512
7	-2.127333	-1.461776	-0.129617

**(Cl, Cl, Cl)**

6	0.000000	0.000000	0.454468
1	0.000000	0.000000	1.540048
17	0.000000	1.705030	-0.083664
17	-1.476599	-0.852515	-0.083664
17	1.476599	-0.852515	-0.083664

**(F, CHO, CCH)**

6	-0.029572	0.431796	0.375304
1	-0.258773	0.465238	1.446686
6	1.212501	-0.290022	0.119261
6	2.221381	-0.908333	-0.117574
1	3.116518	-1.453304	-0.318518
6	-1.193714	-0.252751	-0.362732
8	-1.909803	-1.076222	0.147746
1	-1.301740	0.082556	-1.415309
9	0.050982	1.736795	-0.108931

**(NH<sub>2</sub>, CCH, CCH)**

6	0.241958	0.514164	0.000000
1	1.217821	1.037216	0.000000
6	0.206454	-0.315532	1.218014
6	0.206454	-0.956288	2.239712
1	0.190268	-1.543078	3.130053
6	0.206454	-0.315532	-1.218014
6	0.206454	-0.956288	-2.239712
1	0.190268	-1.543078	-3.130053
7	-0.905958	1.447153	0.000000
1	-0.831651	2.047862	0.820374
1	-0.831651	2.047862	-0.820374

**(NH<sub>2</sub>, CCH, NH<sub>2</sub>)**

6	0.572643	-0.061458	0.000000
1	1.496609	0.531562	0.000000
6	-0.577965	0.857265	0.000000
6	-1.545613	1.577764	0.000000
1	-2.388900	2.230420	0.000000
7	0.572643	-0.810580	1.265340
1	-0.274118	-1.374776	1.331248
1	1.364565	-1.452870	1.278273
7	0.572643	-0.810580	-1.265340
1	1.364565	-1.452870	-1.278273
1	-0.274118	-1.374776	-1.331248

**(NH<sub>2</sub>, CHO, CCH)**

6	0.022079	0.310917	0.490702
1	0.000728	0.415827	1.590518
6	1.376622	-0.085850	0.097209
6	2.464910	-0.467456	-0.259254
1	3.437716	-0.781638	-0.563800
7	-0.376853	1.587802	-0.095297
1	-0.212996	1.548358	-1.100768
1	-1.388770	1.671554	0.009897
6	-0.947031	-0.855304	0.186537
8	-2.010876	-0.690845	-0.361580
1	-0.611182	-1.855798	0.532712

**(NH<sub>2</sub>, CHO, NH<sub>2</sub>)**

6	0.465123	0.018020	0.361418
1	0.590202	-0.027360	1.460555
7	0.419324	1.373087	-0.166099
1	-0.552235	1.681470	-0.205032
1	0.935986	2.022041	0.420999
6	-0.878275	-0.669575	0.107616
8	-1.900920	-0.073752	-0.149056
1	-0.841876	-1.774177	0.193199
7	1.518842	-0.831409	-0.188711
1	1.566624	-0.653725	-1.192645
1	2.420405	-0.540650	0.184845

**(NH<sub>2</sub>, CN, CN)**

6	0.240854	0.497875	0.000000
1	1.222172	1.007592	0.000000
7	-0.919934	1.395457	0.000000
1	-0.879658	1.994786	0.822592
1	-0.879658	1.994786	-0.822592
6	0.212752	-0.348670	1.212787
7	0.212752	-0.969184	2.191719
6	0.212752	-0.348670	-1.212787
7	0.212752	-0.969184	-2.191719

**(NH<sub>2</sub>, F, OH)**

6	0.047382	0.013827	0.354706
1	0.115399	0.094119	1.447921
9	0.146319	1.308364	-0.138284
7	-1.177115	-0.517377	-0.184043
1	-1.401853	-1.402464	0.265227
1	-1.946542	0.129393	-0.026337
8	1.113373	-0.762174	-0.037718

1	0.964663	-0.960263	-0.980451
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**(OH, OH, OH)**

6	0.000000	0.000000	0.328900
1	0.000000	0.000000	1.437961
8	-0.583931	1.169983	-0.152666
1	0.000000	1.908624	0.084212
8	1.305201	-0.079292	-0.152666
1	1.652917	-0.954312	0.084212
8	-0.721270	-1.090691	-0.152666
1	-1.652917	-0.954312	0.084212

**(CH=CH<sub>2</sub>, CH=CH<sub>2</sub>, CH=CH<sub>2</sub>)**

6	0.132864	-0.044143	-0.253352
1	0.341104	0.239679	-1.296135
6	1.467247	-0.228806	0.448346
6	2.660347	-0.107399	-0.132795
1	1.406054	-0.491181	1.505548
1	3.583384	-0.259825	0.420234
1	2.761662	0.152374	-1.184817
6	-0.618217	-1.368715	-0.273421
6	-1.893978	-1.559590	0.063044
1	-0.017857	-2.218019	-0.600984
1	-2.348082	-2.545521	0.011306
1	-2.534164	-0.743096	0.386195
6	-0.648221	1.071649	0.402532
6	-1.071732	2.175221	-0.212999
1	-0.856625	0.937093	1.464904
1	-1.619151	2.950407	0.316740
1	-0.886183	2.348796	-1.271117

**(NH<sub>2</sub>, BH<sub>2</sub>, CCH)**

6	-0.261373	-0.136696	0.580545
1	-0.413955	0.017901	1.647859
6	1.112347	-0.069577	0.166392
6	2.269350	-0.015773	-0.183287
1	3.286807	0.000696	-0.501174
7	-1.197456	0.764887	-0.219549
1	-1.789614	1.381679	0.327767
1	-0.750684	1.246797	-0.993515
5	-1.422982	-0.837719	-0.264744
1	-1.150602	-1.305695	-1.329787
1	-2.406792	-1.174718	0.327512

**(NH<sub>2</sub>, CHO, BH<sub>2</sub>)**

6	-0.314514	-0.590381	-0.437244
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1	-0.598499	-1.181741	-1.303714
6	1.113152	-0.512229	-0.111145
8	1.655118	0.507548	0.290346
1	1.679686	-1.459749	-0.211551
7	-0.963508	0.750798	-0.342830
1	-0.266829	1.455211	-0.088588
1	-1.557838	1.023999	-1.118337
5	-1.408061	-0.333261	0.740240
1	-2.504035	-0.771628	0.551600
1	-1.000400	-0.100095	1.836769

**(NH<sub>2</sub>, CHO, CF<sub>3</sub>)**

6	0.441607	0.323467	-0.547404
1	0.318834	0.340456	-1.640084
6	1.496470	-0.756392	-0.236813
8	2.569831	-0.477516	0.244147
1	1.230112	-1.799275	-0.502318
7	0.779318	1.652820	-0.082504
1	1.002938	1.607858	0.911081
1	1.636877	1.954057	-0.540408
6	-0.919757	-0.096833	0.005928
9	-0.891914	-0.134726	1.357842
9	-1.902306	0.732417	-0.365334
9	-1.240507	-1.339265	-0.429640

**(NH<sub>2</sub>, CHO, CH<sub>3</sub>)**

6	0.437769	0.052897	0.421810
1	0.621397	0.022364	1.508845
6	-0.899711	-0.651587	0.207572
8	-1.869686	-0.125522	-0.292705
1	-0.938805	-1.711492	0.552588
7	0.456175	1.447053	-0.002616
1	0.287488	1.481005	-1.008837
1	-0.347121	1.925038	0.405976
6	1.562361	-0.741007	-0.261285
1	2.526299	-0.275523	-0.039685
1	1.426859	-0.747413	-1.349937
1	1.585634	-1.781000	0.082423

**(NH<sub>2</sub>, CHO, CH=CH<sub>2</sub>)**

6	-0.000899	0.329953	0.391117
1	0.286474	0.362988	1.452182
6	-0.920030	-0.891784	0.222669
8	-2.013924	-0.838202	-0.293179
1	-0.498460	-1.853173	0.592201
7	-0.630173	1.596987	0.030519
1	-1.033891	1.498587	-0.902021

1	-1.435109	1.745797	0.639090
6	1.244963	0.082452	-0.431707
6	2.390911	-0.404817	0.043305
1	1.142856	0.293523	-1.496632
1	3.241525	-0.593359	-0.605656
1	2.529538	-0.622478	1.100334

**(NH<sub>2</sub>, CHO, CHO)**

6	0.010676	0.386980	0.381845
1	0.228982	0.393986	1.463879
6	-0.777638	-0.906278	0.153736
8	-1.922092	-0.912798	-0.237660
1	-0.216766	-1.836081	0.366497
6	1.377605	0.226107	-0.306667
8	2.192211	-0.601972	0.029558
1	1.534741	0.930119	-1.150513
7	-0.706969	1.549512	-0.094295
1	-1.655567	1.271936	-0.345136
1	-0.767418	2.270768	0.616668

**(NH<sub>2</sub>, CHO, CN)**

6	0.063734	0.293588	0.476709
1	0.090283	0.389135	1.575072
6	-0.949210	-0.844669	0.183355
8	-2.014194	-0.625141	-0.337837
1	-0.643903	-1.860142	0.510287
7	-0.279746	1.587404	-0.090892
1	-0.295268	1.514100	-1.107626
1	-1.237461	1.805548	0.182047
6	1.404470	-0.143956	0.054693
7	2.434879	-0.541303	-0.301340

**(NH<sub>2</sub>, CHO, F)**

6	0.506578	0.013159	0.369184
1	0.775210	-0.056592	1.433319
6	-0.877872	-0.607004	0.148889
8	-1.852002	0.041626	-0.154962
1	-0.914396	-1.706742	0.273951
7	0.577328	1.321220	-0.138718
1	-0.312511	1.637888	-0.511873
1	0.985678	2.003242	0.485417
9	1.385388	-0.877364	-0.286503

**(NH<sub>2</sub>, CHO, OH)**

6	0.481298	-0.014121	0.388058
1	0.643936	-0.081873	1.477752

6	-0.894822	-0.632195	0.104290
8	-1.883884	0.014785	-0.159674
1	-0.908831	-1.740173	0.153840
7	0.523905	1.320433	-0.145037
1	-0.421207	1.689944	-0.231577
1	1.086720	1.948408	0.419173
8	1.486820	-0.846781	-0.174195
1	1.589706	-0.525475	-1.087065

**(NH<sub>2</sub>, BH<sub>2</sub>, CH=CH<sub>2</sub>)**

6	0.235598	-0.082849	0.438915
1	0.077013	0.217610	1.474067
7	1.363305	0.751389	-0.176049
1	1.792012	1.432897	0.441445
1	1.164993	1.145061	-1.090529
5	1.573706	-0.840596	0.034527
1	1.594827	-1.431858	-1.008000
1	2.375728	-1.088858	0.888837
6	-1.000463	-0.122800	-0.368334
6	-2.237665	0.020473	0.116930
1	-0.867593	-0.354390	-1.427217
1	-3.114717	-0.095764	-0.513236
1	-2.418753	0.229613	1.169280

**(NH<sub>2</sub>, BH<sub>2</sub>, OH)**

6	0.249532	0.078963	0.513579
1	0.325939	-0.244527	1.550802
7	-0.844688	-0.741929	-0.200451
1	-1.397334	-1.374538	0.369873
1	-0.512664	-1.177824	-1.055316
5	-0.959421	0.883962	-0.073978
1	-0.787445	1.424593	-1.134493
1	-1.853665	1.235393	0.639486
8	1.484804	-0.035364	-0.119471
1	1.559459	0.719737	-0.723016

**(OH, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.289765	-0.220779	0.528806
1	0.129205	-0.553644	1.549172
8	-0.882354	-0.619417	-0.365661
1	-1.589746	-0.983412	0.194512
5	1.594905	-0.021588	-0.183992
1	2.512427	0.386813	0.466506
1	1.695333	-0.160730	-1.364176
5	-0.691365	0.954747	0.003890
1	-0.423853	1.587596	-0.969655
1	-1.520828	1.337594	0.776599

**(OH, BH<sub>2</sub>, CCH)**

6	0.261448	0.062958	0.566920
1	0.411888	-0.286876	1.588971
8	1.151707	-0.775525	-0.381444
1	1.783782	-1.271645	0.167562
5	1.404199	0.874687	-0.150607
1	2.419323	1.057645	0.456278
1	1.161962	1.459895	-1.159144
6	-1.107348	0.031720	0.144316
6	-2.273236	0.040505	-0.173989
1	-3.296797	0.060644	-0.472565

**(OH, BH<sub>2</sub>, OH)**

6	0.239540	-0.206052	0.461184
1	0.364061	0.000629	1.524555
8	-0.773088	0.900881	-0.015574
1	-0.460003	1.151289	-0.904212
5	-1.073565	-0.783015	-0.129965
1	-1.963647	-1.086258	0.604510
1	-1.074402	-1.116989	-1.278437
8	1.401307	-0.178159	-0.262589
1	2.038828	0.420943	0.161605

**(OH, CHO, CCH)**

6	0.020373	0.367003	0.510468
1	0.052717	0.563327	1.596297
8	-0.453330	1.507891	-0.156455
1	-1.201410	1.195258	-0.703703
6	1.359114	-0.060601	0.070524
6	2.445983	-0.443878	-0.288769
1	3.410389	-0.765645	-0.611973
6	-0.937651	-0.813538	0.293201
8	-1.910277	-0.698541	-0.417753
1	-0.679767	-1.761651	0.800493

**(OH, CHO, CHO)**

6	0.017796	0.377124	0.423736
1	0.240930	0.397062	1.505738
8	-0.662616	1.522503	0.008385
1	-1.537536	1.215004	-0.303506
6	-0.809917	-0.879613	0.170659
8	-1.928925	-0.795272	-0.287048
1	-0.332582	-1.843882	0.419784
6	1.367721	0.234868	-0.294883
8	2.172908	-0.620100	-0.010977

1 1.524658 0.980500 -1.101969

**(OH, CHO, OH)**

6 -0.520416 0.021943 0.436477  
8 -0.490130 1.339708 0.002469  
1 0.393172 1.469808 -0.400305  
6 0.866046 -0.611634 0.262877  
8 1.765843 -0.015609 -0.292394  
1 0.972056 -1.659733 0.599386  
8 -1.431505 -0.787126 -0.291336  
1 -1.338519 -0.529849 -1.224782  
1 -0.854159 -0.037870 1.479655

**(NH<sub>2</sub>, BH<sub>2</sub>, COOH)**

6 -0.484062 -0.563769 -0.324185  
1 -0.481664 -1.315838 -1.106812  
6 0.812767 0.072668 -0.028923  
8 0.955289 1.250827 0.253883  
7 -1.558043 0.468750 -0.456612  
1 -1.182530 1.405360 -0.301570  
1 -2.150934 0.398883 -1.277122  
5 -1.660186 -0.548139 0.779545  
1 -2.526416 -1.361849 0.649929  
1 -1.441529 -0.026141 1.830127  
8 1.842479 -0.800677 -0.074080  
1 2.635928 -0.295568 0.184227

**(NH<sub>2</sub>, CHO, COOH)**

6 -0.249004 0.137675 0.593985  
1 -0.196505 -0.067151 1.672330  
6 -1.258552 -0.847501 0.006929  
8 -2.280124 -0.481033 -0.529833  
1 -0.979782 -1.912656 0.093898  
6 1.155036 -0.223304 0.032365  
8 1.651278 -1.310855 0.207254  
7 -0.602980 1.517569 0.280704  
1 -1.495912 1.519306 -0.216666  
1 -0.707066 2.083198 1.117796  
8 1.712382 0.772144 -0.655473  
1 1.046950 1.511048 -0.607541

**(SH, NH<sub>2</sub>, NH<sub>2</sub>)**

7 0.990004 -1.274512 -0.077368  
1 0.870091 -1.343831 -1.087632  
1 1.993811 -1.290584 0.109410  
6 0.466880 -0.010136 0.390578



1	0.526620	0.006337	1.481954
16	-1.350876	0.089419	-0.077149
1	-1.711250	-1.135868	0.363598
7	1.185407	1.149497	-0.098742
1	1.040210	1.266569	-1.101639
1	0.865373	2.002590	0.358000

**(SH, SH, NH<sub>2</sub>)**

7	-0.123480	1.728419	-0.105130
1	0.653182	2.309412	0.207402
1	-0.138273	1.716352	-1.122959
6	-0.025197	0.402611	0.428428
1	-0.006926	0.460657	1.517770
16	1.548251	-0.471575	-0.110218
1	1.417197	-1.582076	0.649835
16	-1.454968	-0.627346	-0.110558
1	-2.402169	0.163788	0.445719

**(SH, SH, SH)**

6	0.000000	0.000000	0.478849
1	0.000000	0.000000	1.568813
16	0.000000	1.735588	-0.131005
1	1.049271	2.154104	0.615437
16	1.503063	-0.867794	-0.131005
1	1.340873	-1.985747	0.615437
16	-1.503063	-0.867794	-0.131005
1	-2.390144	-0.168357	0.615437

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

1	0.399172	0.000002	-1.353784
6	0.460874	-0.000002	-0.247277
6	-0.891692	-0.000004	0.410374
6	-2.062435	0.000000	-0.228543
1	-0.879364	-0.000009	1.500802
1	-3.005600	-0.000003	0.310545
1	-2.124704	0.000004	-1.315512
5	1.366932	1.243099	0.055092
1	2.312469	1.476886	-0.638303
1	1.137837	1.955558	0.988168
5	1.366944	-1.243096	0.055089
1	2.312483	-1.476862	-0.638309
1	1.137844	-1.955557	0.988161

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, CH=CH<sub>2</sub>)**

1	0.176226	-0.057445	-1.387136
6	0.120084	0.137228	-0.313508

6	-1.047645	-0.553574	0.339267
6	-2.286051	-0.594352	-0.198389
1	-0.921082	-0.850095	1.379266
1	-3.135075	-0.961534	0.371298
1	-2.474422	-0.311680	-1.229755
5	-0.785316	1.394476	0.052558
1	-1.427108	1.911287	-0.810520
1	-0.779091	1.848939	1.157202
6	1.432161	-0.035826	0.374117
6	2.595513	-0.269303	-0.236191
1	1.413675	0.071937	1.460208
1	3.523700	-0.353276	0.321692
1	2.665385	-0.375545	-1.316819

**Table S6** Optimized UB3-LYP/6-31G(d) geometries of di- ( $\bullet$ CHXY) and tri- ( $\bullet$ CXYZ) substituted radicals

**(CH<sub>3</sub>, BH<sub>2</sub>, H)**

6	-1.141075	-0.473611	0.000000
1	-1.790996	-0.313732	0.875433
1	-0.810145	-1.516136	0.000000
1	-1.790996	-0.313732	-0.875433
6	0.000000	0.487113	0.000000
1	-0.304464	1.537362	0.000000
5	1.482073	0.117886	0.000000
1	2.321927	0.971161	0.000000
1	1.810760	-1.035364	0.000000

**(CH<sub>3</sub>, CCH, H)**

6	-1.498477	0.833524	0.000000
1	-1.866091	1.379509	0.880891
1	-1.951585	-0.161398	0.000000
1	-1.866091	1.379509	-0.880891
6	0.705479	-0.424403	0.000000
6	1.333972	-1.479339	0.000000
1	1.879088	-2.395165	0.000000
6	0.000000	0.754909	0.000000
1	0.558830	1.689395	0.000000

**(CH<sub>3</sub>, CF<sub>3</sub>, H)**

6	-2.147917	-0.025278	-0.007534
1	-2.425742	-0.226524	1.041084
1	-2.071672	-0.994578	-0.511116
1	-2.972030	0.540525	-0.454172
6	-0.869851	0.730102	-0.095244
1	-0.842547	1.808297	0.020321
6	0.437250	0.034588	-0.012997
9	1.452727	0.840604	-0.390188
9	0.716371	-0.387506	1.252807
9	0.474802	-1.071341	-0.796115

**(CH<sub>3</sub>, CH<sub>3</sub>, H)**

6	-0.011634	-0.197403	1.301139
1	0.973201	-0.646421	1.528957
1	-0.730955	-1.028703	1.296386
1	-0.260173	0.461027	2.141340
6	-0.011634	0.534287	0.000000
1	0.245259	1.591312	0.000000

6	-0.011634	-0.197403	-1.301139
1	-0.730955	-1.028703	-1.296386
1	-0.260173	0.461027	-2.141340
1	0.973201	-0.646421	-1.528957

**(CH<sub>3</sub>, CH=CH<sub>2</sub>, H)**

6	-1.480244	0.669475	0.000000
1	-1.949603	1.133487	0.879598
1	-1.749702	-0.390225	0.000000
1	-1.949603	1.133487	-0.879598
6	0.000000	0.891552	0.000000
1	0.328680	1.929365	0.000000
6	0.983908	-0.094112	0.000000
6	0.802160	-1.467284	0.000000
1	2.014748	0.261584	0.000000
1	1.652676	-2.140785	0.000000
1	-0.182134	-1.924698	0.000000

**(CH<sub>3</sub>, CHO, H)**

6	-1.455837	0.559208	0.000000
1	-1.948018	1.000571	0.878826
1	-1.624264	-0.519990	0.000000
1	-1.948018	1.000571	-0.878826
6	0.000000	0.857594	0.000000
1	0.333646	1.894079	0.000000
6	0.997171	-0.168312	0.000000
8	0.735981	-1.380030	0.000000
1	2.050804	0.174074	0.000000

**(CH<sub>3</sub>, Cl, H)**

6	1.657557	-0.265783	0.008889
1	1.605436	-1.092550	-0.709927
1	1.788541	-0.713944	1.008002
1	2.552502	0.327621	-0.209141
6	0.452746	0.599940	-0.069032
1	0.459628	1.655761	0.173819
17	-1.121642	-0.128343	0.005771

**(CH<sub>3</sub>, CN, H)**

6	1.496327	0.742132	0.000000
1	1.914691	-0.267070	0.000000
1	1.877723	1.277202	0.880995
1	1.877723	1.277202	-0.880995
6	0.000000	0.724244	0.000000
1	-0.544388	1.665050	0.000000
6	-0.746598	-0.445088	0.000000

7	-1.374875	-1.440016	0.000000
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**(CH<sub>3</sub>, F, H)**

6	1.195409	-0.171687	0.012859
1	1.264244	-1.007420	-0.694684
1	1.363648	-0.586150	1.022004
1	2.007917	0.530503	-0.200249
6	-0.114032	0.515197	-0.104575
1	-0.292499	1.526376	0.254950
9	-1.203508	-0.280486	0.018698

**(CH<sub>3</sub>, NH<sub>2</sub>, H)**

6	-1.253376	-0.175938	0.017359
1	-1.460994	-0.498983	1.053990
1	-1.302371	-1.080291	-0.608254
1	-2.074366	0.479550	-0.292242
6	0.060285	0.520642	-0.128741
1	0.137109	1.561542	0.179489
7	1.224146	-0.232369	0.114013
1	1.208724	-1.151526	-0.321123
1	2.081422	0.248072	-0.141655

**(CH<sub>3</sub>, OH, H)**

6	-1.229238	-0.163516	0.011264
1	-1.420584	-0.556838	1.025477
1	-1.294998	-1.014321	-0.678710
1	-2.034470	0.538292	-0.230488
6	0.092622	0.508185	-0.105133
1	0.229194	1.524256	0.269615
8	1.169488	-0.342312	0.025038
1	1.984649	0.179090	-0.022983

**(CH<sub>3</sub>, SH, H)**

6	-1.687038	-0.251218	0.036873
1	-1.862590	-0.550416	1.084497
1	-1.626605	-1.177188	-0.551530
1	-2.572787	0.299798	-0.299027
6	-0.461183	0.585588	-0.123868
1	-0.504504	1.659085	0.031000
16	1.159719	-0.057764	0.040533
1	0.900307	-1.313283	-0.391493

**(F, BH<sub>2</sub>, H)**

6	0.000000	0.459124	0.000000
1	-0.212076	1.529230	0.000000

9	-1.139443	-0.239270	0.000000
5	1.346589	-0.231592	0.000000
1	1.407853	-1.422889	0.000000
1	2.326267	0.450306	0.000000

**(F, CCH, H)**

6	0.605235	-0.496363	0.000000
1	1.673307	-0.674330	0.000000
9	-0.135357	-1.621854	0.000000
6	0.000000	0.731325	0.000000
6	-0.519031	1.842302	0.000000
1	-0.972321	2.807434	0.000000

**(F, CF<sub>3</sub>, H)**

6	-0.929212	0.695817	-0.144528
1	-1.063944	1.738118	0.122129
9	-1.996270	-0.090259	0.005186
6	0.389780	0.018555	-0.013534
9	0.642340	-0.399474	1.251457
9	1.363500	0.884944	-0.357035
9	0.468269	-1.064583	-0.807803

**(F, CH=CH<sub>2</sub>, H)**

6	-0.902985	-0.130465	0.000000
1	-1.983174	-0.041585	0.000000
9	-0.477651	-1.408017	0.000000
6	0.000000	0.911664	0.000000
6	1.378333	0.778465	0.000000
1	-0.442542	1.906068	0.000000
1	2.024416	1.648668	0.000000
1	1.848075	-0.198981	0.000000

**(F, CHO, H)**

6	0.000000	0.661232	0.000000
1	-0.825141	1.366133	0.000000
9	1.214791	1.202671	0.000000
6	-0.142109	-0.750429	0.000000
8	-1.256994	-1.290576	0.000000
1	0.800624	-1.330383	0.000000

**(F, Cl, H)**

6	-0.553025	0.550106	-0.135266
1	-0.725145	1.499421	0.368032
9	-1.530035	-0.342330	0.027876
17	1.047859	-0.101123	0.011334

**(F, CN, H)**

6	0.000000	0.752527	0.000000
1	-0.537455	1.691461	0.000000
9	1.330493	0.846359	0.000000
6	-0.594352	-0.498605	0.000000
7	-1.124410	-1.547461	0.000000

**(F, F, H)**

6	-0.030417	0.508003	0.000000
1	0.730013	1.293239	0.000000
9	-0.030417	-0.241181	1.103440
9	-0.030417	-0.241181	-1.103440

**(F, NH<sub>2</sub>, H)**

6	0.052941	0.497580	0.176981
1	0.120397	1.492213	-0.270134
9	1.169172	-0.249031	-0.040920
7	-1.118601	-0.211854	-0.122410
1	-1.178385	-1.094671	0.380534
1	-1.951994	0.341231	0.052867

**(F, OH, H)**

6	-0.016318	0.497910	0.180668
1	-0.066599	1.479850	-0.290485
9	-1.125667	-0.255829	-0.045039
8	1.148430	-0.141533	-0.086188
1	1.108069	-1.032588	0.301333

**(F, SH, H)**

6	-0.562666	0.522375	0.202012
1	-0.774313	1.552135	-0.076851
9	-1.567649	-0.332605	-0.080040
16	1.079144	-0.033664	-0.068729
1	0.992839	-1.154315	0.684813

**(Cl, BH<sub>2</sub>, H)**

6	0.000000	0.782025	0.000000
1	-0.801823	1.516378	0.000000
17	-0.633972	-0.824399	0.000000
5	1.491291	1.077720	0.000000
1	2.291697	0.193905	0.000000
1	1.831189	2.223740	0.000000

**(Cl, CCH, H)**

6	0.000000	0.717863	0.000000
1	-0.164858	1.787524	0.000000
17	-1.455294	-0.231190	0.000000
6	1.239049	0.138051	0.000000
6	2.357138	-0.364433	0.000000
1	3.327731	-0.806184	0.000000

**(Cl, CF<sub>3</sub>, H)**

6	-0.495295	0.786834	-0.063657
1	-0.500896	1.858893	0.078553
17	-1.984554	-0.039138	0.001436
6	0.779494	0.018042	-0.007863
9	0.999749	-0.534643	1.208402
9	1.806596	0.852045	-0.268146
9	0.808445	-0.986602	-0.904016

**(Cl, CH=CH<sub>2</sub>, H)**

6	0.000000	0.885293	0.000000
1	-0.246616	1.939043	0.000000
17	-1.395565	-0.150199	0.000000
6	1.303407	0.407862	0.000000
6	1.717931	-0.908249	0.000000
1	2.062978	1.189661	0.000000
1	2.773146	-1.157242	0.000000
1	1.007066	-1.727510	0.000000

**(Cl, CHO, H)**

6	0.000000	0.511098	0.000000
1	0.048409	1.594195	0.000000
17	-1.565557	-0.186942	0.000000
6	1.181805	-0.296711	0.000000
8	2.305414	0.211343	0.000000
1	1.031919	-1.393244	0.000000

**(Cl, Cl, H)**

6	0.012055	0.695351	0.000000
1	-0.482212	1.658778	0.000000
17	0.012055	-0.171497	1.485148
17	0.012055	-0.171497	-1.485148

**(Cl, CN, H)**

6	0.000000	0.706071	0.000000
1	-0.160671	1.776243	0.000000



17	-1.405969	-0.279531	0.000000
6	1.268169	0.149053	0.000000
7	2.350446	-0.307852	0.000000

**(Cl, NH<sub>2</sub>, H)**

6	-0.517511	0.572933	0.172935
1	-0.609112	1.568730	-0.252732
17	1.097435	-0.108964	-0.019699
7	-1.562215	-0.302415	-0.116663
1	-1.532520	-1.173944	0.405587
1	-2.474190	0.136912	-0.038939

**(Cl, OH, H)**

6	-0.558985	0.566993	0.171347
1	-0.675492	1.546387	-0.283226
17	1.073094	-0.105410	-0.018862
8	-1.596030	-0.255132	-0.094727
1	-1.444960	-1.115317	0.333610

**(Cl, SH, H)**

6	-0.004477	0.676222	0.170998
1	-0.041605	1.732072	-0.070130
17	-1.513765	-0.166628	-0.031613
16	1.533806	-0.107369	-0.065195
1	1.261573	-1.238808	0.624693

**(NH<sub>2</sub>, BH<sub>2</sub>, H)**

7	-1.100049	-0.326036	0.000000
1	-2.043487	0.033088	0.000000
1	-0.991237	-1.330960	0.000000
6	0.000000	0.471885	0.000000
1	-0.254631	1.531543	0.000000
5	1.411039	-0.050423	0.000000
1	1.598760	-1.239067	0.000000
1	2.335744	0.708452	0.000000

**(NH<sub>2</sub>, CCH, H)**

7	1.609052	-0.371808	-0.089717
1	2.477524	-0.064982	0.333719
1	1.377534	-1.324020	0.169997
6	0.552613	0.534248	0.012717
1	0.827818	1.583442	-0.018177
6	-0.770050	0.147362	-0.008086
6	-1.946640	-0.198451	0.036902
1	-2.961779	-0.490742	-0.106716

**(NH<sub>2</sub>, CF<sub>3</sub>, H)**

7	-2.063824	0.016730	-0.058775
1	-2.850808	-0.351314	0.460587
1	-1.962728	1.021371	0.008329
6	-0.897247	-0.721665	-0.073612
1	-0.945508	-1.787821	0.095061
6	0.404986	-0.040755	-0.012199
9	0.342889	1.186019	-0.599957
9	0.857189	0.191600	1.261249
9	1.373187	-0.758154	-0.621035

**(NH<sub>2</sub>, CH=CH<sub>2</sub>, H)**

7	1.464380	-0.505150	-0.077469
1	2.405925	-0.387951	0.275074
1	1.046541	-1.367559	0.252557
6	0.653653	0.618751	-0.002122
1	1.183483	1.565083	-0.034703
6	-0.741551	0.591999	0.013709
6	-1.556358	-0.523970	-0.004355
1	-1.219404	1.569517	0.047441
1	-2.635631	-0.427972	0.035936
1	-1.166036	-1.535746	-0.077416

**(NH<sub>2</sub>, CHO, H)**

7	1.363824	-0.450024	-0.046043
1	2.344227	-0.420876	0.186439
1	0.870805	-1.331634	0.049385
6	0.583387	0.657440	0.004285
1	1.065543	1.628610	0.010166
6	-0.829400	0.494200	0.000771
8	-1.364787	-0.631999	0.006204
1	-1.432971	1.420219	-0.003654

**(NH<sub>2</sub>, CN, H)**

7	1.560369	-0.347036	-0.078383
1	2.452134	-0.019332	0.270415
1	1.367385	-1.312621	0.158070
6	0.502430	0.539365	0.017159
1	0.734892	1.596395	-0.015832
6	-0.820051	0.112708	0.000140
7	-1.938752	-0.249661	0.004605

**(NH<sub>2</sub>, NH<sub>2</sub>, H)**

7	1.171862	-0.257571	-0.061537
1	2.002678	0.302813	-0.217773
1	1.284485	-0.773422	0.817850

6	-0.003993	0.524186	-0.106339
1	-0.036072	1.517859	0.355404
7	-1.172876	-0.235903	0.093821
1	-2.020951	0.309760	-0.023536
1	-1.199083	-1.047807	-0.519895

**(NH<sub>2</sub>, OH, H)**

7	1.122266	-0.264314	-0.042686
1	1.933604	0.227018	-0.404991
1	1.348680	-0.613126	0.895430
6	-0.044203	0.527995	-0.096040
1	-0.120526	1.510740	0.375092
8	-1.213454	-0.173934	0.044122
1	-1.044770	-1.050936	-0.343458

**(NH<sub>2</sub>, SH, H)**

7	-1.597398	-0.304646	0.082001
1	-2.505373	0.106482	-0.113091
1	-1.476638	-1.196426	-0.388129
6	-0.520272	0.567091	-0.047362
1	-0.691362	1.589674	0.273476
16	1.107950	-0.076936	-0.079098
1	1.249594	-0.538781	1.203482

**(OH, BH<sub>2</sub>, H)**

6	0.000000	0.482124	0.000000
1	-0.198979	1.552830	0.000000
8	-1.169022	-0.186674	0.000000
1	-0.971837	-1.141358	0.000000
5	1.353739	-0.180378	0.000000
1	2.351941	0.473459	0.000000
1	1.402359	-1.382392	0.000000

**(OH, CCH, H)**

6	0.648400	-0.463579	0.000000
1	1.725410	-0.570760	0.000000
8	0.000075	-1.667258	0.000000
1	-0.957050	-1.499102	0.000000
6	0.000000	0.748505	0.000000
6	-0.593133	1.823006	0.000000
1	-1.100565	2.760333	0.000000

**(OH, CF<sub>3</sub>, H)**

6	-0.906226	-0.741229	-0.129549
1	-0.981488	-1.794014	0.107901
8	-2.047630	-0.031744	0.043557
1	-1.859970	0.902152	-0.158694

6	0.393680	-0.039745	-0.011904
9	0.274505	1.223936	-0.514750
9	0.840412	0.106301	1.264697
9	1.362614	-0.682275	-0.688719

**(OH, CH=CH<sub>2</sub>, H)**

6	0.000000	0.916647	0.000000
1	-0.304832	1.956324	0.000000
8	1.353320	0.796466	0.000000
1	1.589428	-0.145454	0.000000
6	-0.907392	-0.134493	0.000000
6	-0.617325	-1.488812	0.000000
1	-1.953116	0.166226	0.000000
1	-1.408084	-2.229600	0.000000
1	0.398344	-1.879277	0.000000

**(OH, CHO, H)**

6	0.000000	0.902125	0.000000
1	-0.239331	1.958708	0.000000
8	1.296573	0.602124	0.000000
1	1.309810	-0.387341	0.000000
6	-0.923957	-0.176894	0.000000
8	-0.487182	-1.348293	0.000000
1	-2.001867	0.046599	0.000000

**(OH, CN, H)**

6	0.000000	0.763648	0.000000
1	-0.532128	1.704607	0.000000
8	1.349597	0.891513	0.000000
1	1.762801	0.011294	0.000000
6	-0.642198	-0.466111	0.000000
7	-1.167751	-1.519033	0.000000

**(OH, OH, H)**

6	0.005390	0.510762	0.152701
1	0.010721	1.489085	-0.340042
8	1.183111	-0.144584	-0.052751
1	1.062764	-1.056054	0.263843
8	-1.087887	-0.306779	-0.090270
1	-1.867619	0.113304	0.304154

**(OH, SH, H), H)**

6	-0.542912	0.521350	0.189795
1	-0.715731	1.566112	-0.068356
8	-1.538289	-0.382654	-0.097574

1	-2.392394	0.046464	0.075659
16	1.102141	-0.034927	-0.068990
1	1.037650	-1.120608	0.738359

**(SH, BH<sub>2</sub>, H)**

6	0.000000	0.786275	0.000000
1	-0.779732	1.547030	0.000000
16	-0.699687	-0.793780	0.000000
1	0.449205	-1.506371	0.000000
5	1.479921	1.099560	0.000000
1	1.845153	2.237970	0.000000
1	2.280764	0.206406	0.000000

**(SH, CCH, H)**

6	0.000000	0.726442	0.000000
1	-0.147079	1.801281	0.000000
16	-1.502182	-0.188167	0.000000
1	-0.946738	-1.418069	0.000000
6	1.256907	0.171965	0.000000
6	2.373213	-0.333115	0.000000
1	3.348009	-0.764286	0.000000

**(SH, CF<sub>3</sub>, H)**

6	-0.489285	-0.773570	-0.154164
1	-0.457964	-1.850088	-0.043986
16	-2.042501	-0.029514	0.019458
1	-1.646559	1.234870	-0.238391
6	0.786861	-0.031484	-0.011792
9	0.731530	1.191177	-0.596725
9	1.136838	0.185957	1.283677
9	1.798196	-0.719604	-0.579531

**(SH, CH=CH<sub>2</sub>, H)**

6	0.000000	0.474036	0.000000
1	0.105572	1.555260	0.000000
16	-1.677899	-0.039032	0.000000
1	-1.454983	-1.371521	0.000000
6	1.124188	-0.351550	0.000000
6	2.428099	0.096316	0.000000
1	0.957112	-1.429715	0.000000
1	3.260322	-0.598939	0.000000
1	2.664642	1.156613	0.000000

**(SH, CHO, H)**

6	0.000000	0.889988	0.000000
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1	-0.181253	1.959077	0.000000
16	-1.373183	-0.147384	0.000000
1	-0.604088	-1.268599	0.000000
6	1.329342	0.351442	0.000000
8	1.579519	-0.859920	0.000000
1	2.144069	1.098443	0.000000

**(SH, CN, H)**

6	0.000000	0.716863	0.000000
1	-0.157133	1.789093	0.000000
16	-1.453327	-0.246620	0.000000
1	-0.856086	-1.456933	0.000000
6	1.284083	0.193990	0.000000
7	2.365993	-0.264480	0.000000

**(SH, SH, H)**

6	-0.002955	0.692784	0.103901
1	-0.006903	1.746500	-0.155309
16	-1.551096	-0.103215	-0.045249
1	-1.270131	-1.187693	0.715876
16	1.488542	-0.231407	-0.065281
1	2.295631	0.638438	0.584511

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, H)**

6	0.004584	-0.741269	0.000000
1	-0.980911	-1.213897	0.000000
6	0.000000	0.666139	0.000000
6	-1.135190	1.445163	0.000000
1	0.967167	1.169474	0.000000
1	-1.085980	2.529822	0.000000
1	-2.124797	0.994834	0.000000
5	1.283605	-1.578983	0.000000
1	1.239965	-2.774922	0.000000
1	2.350168	-1.030595	0.000000

**(CH=CH<sub>2</sub>, CCH, H)**

6	0.000000	0.512594	0.000000
1	-0.286894	1.563637	0.000000
6	1.361300	0.212330	0.000000
6	2.556499	-0.033267	0.000000
1	3.598820	-0.256870	0.000000
6	-1.021871	-0.463885	0.000000
6	-2.358989	-0.176029	0.000000
1	-0.708681	-1.506706	0.000000
1	-3.107869	-0.960868	0.000000
1	-2.717004	0.850346	0.000000

**(CH=CH<sub>2</sub>, CF<sub>3</sub>, H)**

6	0.565537	-0.530910	-0.000013
6	-0.836096	-0.030833	-0.000002
1	0.665302	-1.612502	-0.000010
6	1.673548	0.299725	-0.000005
6	2.983621	-0.149128	0.000003
1	1.495231	1.372721	-0.000008
1	3.816551	0.545360	0.000009
1	3.218295	-1.209869	0.000006
9	-0.907327	1.318223	-0.000107
9	-1.519356	-0.471735	1.085221
9	-1.519432	-0.471913	-1.085102

**(CH=CH<sub>2</sub>, CH=CH<sub>2</sub>, H)**

6	0.000000	0.692534	0.000000
1	0.317546	1.734145	0.000000
6	1.029416	-0.285442	0.000000
6	2.360096	0.003481	0.000000
1	0.733784	-1.333965	0.000000
1	3.113389	-0.777745	0.000000
1	2.716654	1.030849	0.000000
6	-1.397590	0.445990	0.000000
6	-2.032379	-0.765389	0.000000
1	-2.028660	1.334504	0.000000
1	-3.115761	-0.826181	0.000000
1	-1.494208	-1.708648	0.000000

**(CH=CH<sub>2</sub>, CHO, H)**

6	0.000000	0.321316	0.000000
1	0.103494	1.404419	0.000000
6	1.132523	-0.503727	0.000000
6	2.428508	-0.047201	0.000000
1	0.963623	-1.581390	0.000000
1	3.271920	-0.729847	0.000000
1	2.650904	1.016432	0.000000
6	-1.345130	-0.211093	0.000000
8	-2.358428	0.481985	0.000000
1	-1.417926	-1.321260	0.000000

**(CH=CH<sub>2</sub>, CN, H)**

6	0.000000	0.514056	0.000000
1	-0.329663	1.550285	0.000000
6	-0.946878	-0.525180	0.000000
6	-2.303135	-0.316691	0.000000
1	-0.570668	-1.546216	0.000000

1	-3.001788	-1.146160	0.000000
1	-2.721244	0.686289	0.000000
6	1.386990	0.284400	0.000000
7	2.543072	0.102328	0.000000

**(CCH, BH<sub>2</sub>, H)**

6	0.658412	-0.510445	0.000000
1	1.748845	-0.455073	0.000000
6	0.000000	0.702761	0.000000
6	-0.588850	1.779829	0.000000
1	-1.118528	2.705634	0.000000
5	-0.069856	-1.861622	0.000000
1	0.565674	-2.874493	0.000000
1	-1.264082	-1.900826	0.000000

**(CCH, CCH, H)**

6	0.000000	0.000000	0.754098
1	0.000000	0.000000	1.843423
6	0.000000	1.225742	0.094579
6	0.000000	2.310583	-0.464659
1	0.000000	3.252879	-0.963526
6	0.000000	-1.225742	0.094579
6	0.000000	-2.310583	-0.464659
1	0.000000	-3.252879	-0.963526

**(CCH, CF<sub>3</sub>, H)**

6	-0.508133	-0.835263	-0.006502
6	0.727846	0.005299	-0.002903
1	-0.348362	-1.908972	0.020582
6	-1.768228	-0.303989	0.000690
6	-2.906659	0.154005	0.000020
1	-3.889435	0.568618	0.005616
9	1.582806	-0.397189	-0.971941
9	0.464219	1.308821	-0.196623
9	1.393958	-0.109405	1.171451

**(CCH, CHO, H)**

6	0.000000	0.557216	0.000000
1	-0.226390	1.621226	0.000000
6	1.311482	0.124834	0.000000
6	2.470563	-0.269284	0.000000
1	3.479565	-0.616034	0.000000
6	-1.124529	-0.362007	0.000000
8	-2.291437	0.016260	0.000000
1	-0.866771	-1.439829	0.000000



**(CCH, CN, H)**

6	0.000000	0.747542	0.000000
1	0.022581	1.835019	0.000000
6	1.185396	0.034310	0.000000
6	2.242992	-0.578041	0.000000
1	3.159795	-1.123822	0.000000
6	-1.258472	0.122890	0.000000
7	-2.314554	-0.381629	0.000000

**(CF<sub>3</sub>, BH<sub>2</sub>, H)**

6	-0.979962	-0.672532	-0.000714
6	0.362704	-0.012915	-0.002001
1	-0.890262	-1.758158	0.015769
9	0.299240	1.326805	-0.086420
9	1.037793	-0.320064	1.132318
9	1.107754	-0.453564	-1.043751
5	-2.336418	0.050751	-0.002866
1	-2.392389	1.240137	0.030270
1	-3.334796	-0.601653	-0.034740

**(CF<sub>3</sub>, CF<sub>3</sub>, H)**

6	-1.302456	-0.004015	0.085632
6	0.000000	-0.000366	0.809724
6	1.302458	0.003939	0.085641
1	-0.000009	-0.000865	1.891818
9	-2.264492	-0.541078	0.862658
9	-1.695391	1.247761	-0.238518
9	-1.238610	-0.715982	-1.056246
9	1.238800	0.717498	-1.055260
9	2.264633	0.539684	0.863401
9	1.695060	-1.247492	-0.240235

**(CF<sub>3</sub>, CHO, H)**

6	0.704428	0.013047	-0.001998
6	-0.435478	0.990187	-0.009582
1	-0.182138	2.045508	0.005440
6	-1.806290	0.566387	-0.004889
8	-2.152323	-0.617501	0.002034
1	-2.557994	1.378520	-0.005015
9	1.879416	0.673847	-0.093060
9	0.727668	-0.706427	1.136485
9	0.635444	-0.845391	-1.034301

**(CF<sub>3</sub>, CN, H)**

6	-0.183915	0.687594	0.000000
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6	-0.652989	-0.736587	0.000000
1	-1.724208	-0.906345	0.000000
6	0.225596	-1.802300	0.000000
7	0.965852	-2.716124	0.000000
9	1.153878	0.775529	0.000000
9	-0.652989	1.335956	1.086196
9	-0.652989	1.335956	-1.086196

**(BH<sub>2</sub>, BH<sub>2</sub>, H)**

6	0.008557	0.495411	0.000000
1	-0.140902	1.581680	0.000000
5	0.008557	-0.237740	1.336823
1	0.763383	-1.149297	1.526052
1	-0.761390	0.060927	2.205967
5	0.008557	-0.237740	-1.336823
1	0.763383	-1.149297	-1.526052
1	-0.761390	0.060927	-2.205967

**(BH<sub>2</sub>, CHO, H)**

6	-0.555871	-0.450206	-0.015296
1	-0.355987	-1.522158	-0.044966
5	-1.981544	0.143564	0.002876
1	-2.125055	1.328213	-0.075637
1	-2.935671	-0.566147	0.100520
6	0.648192	0.363799	0.007134
8	1.783764	-0.112590	0.003966
1	0.500392	1.461431	0.022952

**(BH<sub>2</sub>, CN, H)**

6	0.629024	-0.487841	0.000000
1	1.718512	-0.451702	0.000000
6	0.000000	0.755916	0.000000
7	-0.544665	1.798336	0.000000
5	-0.156191	-1.818578	0.000000
1	-1.347882	-1.805814	0.000000
1	0.448831	-2.846392	0.000000

**(CHO, CHO, H)**

6	0.000000	0.712011	0.000000
1	0.312163	1.753648	0.000000
6	-1.408337	0.375776	0.000000
8	-1.819450	-0.785411	0.000000
1	-2.118757	1.224595	0.000000
6	1.040252	-0.302135	0.000000
8	2.233429	-0.007044	0.000000
1	0.703272	-1.352516	0.000000

**(CHO, CN, H)**

6	0.000000	0.549065	0.000000
1	-0.271081	1.601192	0.000000
6	-1.066380	-0.439943	0.000000
8	-2.247448	-0.113130	0.000000
1	-0.754431	-1.500834	0.000000
6	1.346996	0.186532	0.000000
7	2.474486	-0.138463	0.000000

**(CN, CN, H)**

6	0.000000	0.000000	0.731738
1	0.000000	0.000000	1.818418
6	0.000000	1.223409	0.055198
7	0.000000	2.259948	-0.490802
6	0.000000	-1.223409	0.055198
7	0.000000	-2.259948	-0.490802

**(COOH, BH<sub>2</sub>, H)**

6	0.809259	-0.652646	-0.038461
1	0.696141	-1.733943	-0.107358
6	-0.459958	0.088852	-0.003999
8	-0.565652	1.303983	0.009739
8	-1.542161	-0.735217	0.012381
1	-2.325564	-0.154511	0.038383
5	2.189156	0.030674	0.015454
1	3.155728	-0.634459	0.241416
1	2.294613	1.202185	-0.171912

**(COOH, CCH, H)**

6	0.000000	0.816025	0.000000
1	-0.533627	1.761920	0.000000
6	-0.785506	-0.421331	0.000000
8	-0.342552	-1.554294	0.000000
8	-2.120551	-0.150420	0.000000
1	-2.565768	-1.017702	0.000000
6	1.375422	0.799007	0.000000
6	2.599721	0.820148	0.000000
1	3.666396	0.810403	0.000000

**(COOH, CF<sub>3</sub>, H)**

6	-0.095715	0.798025	0.000000
1	0.102626	1.862729	0.000000
6	-1.461275	0.295629	0.000000
8	-1.774346	-0.881936	0.000000

8	-2.365082	1.309200	0.000000
1	-3.245160	0.888538	0.000000
6	1.066722	-0.143496	0.000000
9	1.066722	-0.937104	1.088221
9	2.222063	0.555282	0.000000
9	1.066722	-0.937104	-1.088221

**(COOH, CH<sub>3</sub>, H)**

6	-0.549095	-0.787629	0.000000
1	-1.629690	-0.894531	0.000000
6	0.000000	0.552443	0.000000
8	1.192352	0.831006	0.000000
8	-0.968935	1.514499	0.000000
1	-0.493564	2.365259	0.000000
6	0.329478	-1.983635	0.000000
1	0.136144	-2.616457	0.878907
1	1.381335	-1.688934	0.000000
1	0.136144	-2.616457	-0.878907

**(COOH, CH=CH<sub>2</sub>, H)**

6	-0.898778	-0.286523	0.000000
1	-1.959515	-0.058563	0.000000
6	0.000000	0.867400	0.000000
8	1.220915	0.855843	0.000000
8	-0.702973	2.036631	0.000000
1	-0.032450	2.744459	0.000000
6	-0.490055	-1.625267	0.000000
6	0.805138	-2.100824	0.000000
1	-1.295165	-2.359327	0.000000
1	0.994396	-3.169700	0.000000
1	1.651363	-1.425380	0.000000

**(COOH, CHO, H)**

6	0.000000	0.632667	0.000000
1	-0.491151	1.600371	0.000000
6	-0.799628	-0.593979	0.000000
8	-0.335296	-1.722052	0.000000
8	-2.129975	-0.339298	0.000000
1	-2.576981	-1.206790	0.000000
6	1.441744	0.579446	0.000000
8	2.130066	1.601765	0.000000
1	1.897069	-0.425704	0.000000

**(COOH, Cl, H)**

6	0.000000	0.805429	0.000000
1	0.337484	1.832963	0.000000

6	0.983996	-0.257894	0.000000
8	2.183372	-0.022397	0.000000
8	0.466727	-1.509249	0.000000
1	1.232218	-2.112509	0.000000
17	-1.686733	0.543971	0.000000

**(COOH, CN, H)**

6	0.000000	0.824201	0.000000
1	-0.534427	1.768439	0.000000
6	-0.750336	-0.438634	0.000000
8	-0.255310	-1.547678	0.000000
8	-2.085451	-0.205148	0.000000
1	-2.517489	-1.079701	0.000000
6	1.389937	0.828319	0.000000
7	2.562914	0.864364	0.000000

**(COOH, F, H)**

6	0.771671	-0.652412	0.000029
1	0.968981	-1.716675	0.000150
6	-0.560560	-0.106253	0.000007
8	-1.556885	-0.815727	-0.000031
8	-0.592384	1.250175	0.000026
1	-1.536662	1.492132	-0.000029
9	1.832796	0.144550	-0.000034

**(COOH, NH<sub>2</sub>, H)**

6	0.714550	-0.680237	0.011896
1	0.735124	-1.761454	0.010788
6	-0.501389	0.074026	0.002453
8	-0.551849	1.304879	0.008467
8	-1.624767	-0.705462	-0.003447
1	-2.368939	-0.077276	0.002029
7	1.888193	0.012039	-0.065187
1	1.804578	1.014307	0.067620
1	2.745853	-0.417917	0.249614

**(COOH, OH, H)**

6	-0.610814	-0.813645	0.000000
1	-1.671037	-1.022937	0.000000
6	0.000000	0.482779	0.000000
8	1.226520	0.617098	0.000000
8	-0.869540	1.523005	0.000000
1	-0.322795	2.329579	0.000000
8	0.210641	-1.869373	0.000000
1	1.117750	-1.487291	0.000000

**(COOH, SH, H)**

6	0.000000	0.790136	0.000000
1	0.420906	1.787220	0.000000
6	0.846492	-0.381511	0.000000
8	0.449838	-1.541181	0.000000
8	2.169227	-0.060361	0.000000
1	2.646565	-0.910150	0.000000
16	-1.713140	0.637575	0.000000
1	-1.688700	-0.717695	0.000000

**(COOH, COOH, H)**

6	0.000000	0.777124	0.000000
1	0.066623	1.857940	0.000000
6	1.216715	-0.022624	0.000000
8	1.232859	-1.253723	0.000000
8	2.341259	0.714698	0.000000
1	3.091826	0.090364	0.000000
6	-1.355128	0.192109	0.000000
8	-2.330279	0.923233	0.000000
8	-1.464459	-1.144673	0.000000
1	-0.563017	-1.544250	0.000000

**(BH<sub>2</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	0.000000	0.000000	0.696060
5	0.000000	0.000000	2.236595
1	0.364822	0.967385	2.825539
1	-0.364822	-0.967385	2.825539
6	0.793171	0.998131	-0.108429
9	1.801386	1.516413	0.616694
9	1.329180	0.443682	-1.213409
9	0.000000	2.018584	-0.498244
6	-0.793171	-0.998131	-0.108429
9	0.000000	-2.018584	-0.498244
9	-1.801386	-1.516413	0.616694
9	-1.329180	-0.443682	-1.213409

**(BH<sub>2</sub>, BH<sub>2</sub>, CF<sub>3</sub>)**

6	0.967259	0.000000	-0.076706
5	1.712675	-1.335144	0.023173
1	1.323047	-2.201621	0.747935
1	2.719858	-1.495261	-0.600117
5	1.712675	1.335142	0.023173
1	1.323055	2.201616	0.747942
1	2.719854	1.495265	-0.600124
6	-0.535247	0.000000	-0.026885
9	-1.069403	-1.087457	-0.625145

9	-0.950599	-0.000006	1.260742
9	-1.069402	1.087464	-0.625133

**(BH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000001	-0.085417	-0.000002
5	-1.381599	-0.709101	0.076877
1	-2.180138	-0.469646	-0.784980
1	-1.713256	-1.394563	1.000580
5	1.381606	-0.709089	-0.076878
1	2.180137	-0.469635	0.784988
1	1.713275	-1.394541	-1.000583
5	-0.000007	1.446686	0.000001
1	-0.714596	2.049200	-0.747228
1	0.714576	2.049205	0.747231

**(CF<sub>3</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	0.000243	-0.000271	-0.001276
6	-0.082465	1.501338	-0.000422
9	-1.358425	1.918319	0.001950
9	0.526377	2.010106	1.087726
9	0.523026	2.012030	-1.089139
6	1.342435	-0.679408	-0.000420
9	1.479336	-1.463483	-1.086154
9	2.341658	0.216638	-0.003948
9	1.480581	-1.456341	1.090653
6	-1.259810	-0.822279	-0.000467
9	-0.984418	-2.135630	-0.009237
9	-1.998859	-0.556801	1.093461
9	-2.009543	-0.544425	-1.083588

**(NH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000000	0.000000	-0.076214
7	0.000000	0.000000	1.287424
1	0.000000	0.864171	1.815824
1	0.000000	-0.864171	1.815824
5	0.000000	-1.355523	-0.791978
1	0.000000	-2.373368	-0.149293
1	0.000000	-1.412339	-1.983984
5	0.000000	1.355523	-0.791978
1	0.000000	2.373368	-0.149293
1	0.000000	1.412339	-1.983984

**(NH<sub>2</sub>, CF<sub>3</sub>, BH<sub>2</sub>)**

6	0.936460	0.057672	-0.021998
7	1.494489	-1.180081	0.016653
1	0.938246	-2.016475	-0.096931

1	2.500286	-1.271298	0.001472
6	-0.569797	0.041247	-0.004017
9	-1.065924	-1.156925	-0.429846
9	-1.092529	0.994290	-0.792408
9	-1.060808	0.236104	1.241503
5	1.744844	1.330866	-0.007332
1	1.208294	2.394471	-0.016953
1	2.940906	1.244813	0.015346

**(NH<sub>2</sub>, CF<sub>3</sub>, CF<sub>3</sub>)**

6	0.000927	0.575244	-0.212227
7	0.009237	1.931802	0.034694
1	0.859607	2.421137	-0.215717
1	-0.843757	2.427896	-0.191065
6	-1.291929	-0.142546	-0.026125
9	-1.388930	-1.223487	-0.820741
9	-2.324057	0.690937	-0.322859
9	-1.491858	-0.573629	1.244555
6	1.289844	-0.148108	-0.026918
9	2.316727	0.626210	-0.470018
9	1.315199	-1.308698	-0.704554
9	1.564746	-0.442354	1.268675

**(NH<sub>2</sub>, NH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000000	0.000000	0.084850
7	0.000000	1.155424	-0.672356
1	-0.474066	1.128550	-1.569534
1	-0.187286	2.000315	-0.149365
7	0.000000	-1.155424	-0.672356
1	0.474066	-1.128550	-1.569534
1	0.187286	-2.000315	-0.149365
5	0.000000	0.000000	1.595127
1	0.101031	-1.040614	2.183022
1	-0.101031	1.040614	2.183022

**(NH<sub>2</sub>, NH<sub>2</sub>, CF<sub>3</sub>)**

6	0.862899	0.007712	-0.243868
7	1.607126	-1.170195	-0.062656
1	1.937382	-1.303865	0.896963
1	1.091619	-1.991462	-0.360285
7	1.540709	1.185934	0.078135
1	2.470533	1.216287	-0.329561
1	1.015453	2.026197	-0.138255
6	-0.606461	0.002639	-0.018994
9	-1.182965	-1.045867	-0.658954
9	-1.178653	1.145199	-0.476533
9	-0.981544	-0.112603	1.291037



**(NH<sub>2</sub>, NH<sub>2</sub>, NH<sub>2</sub>)**

6	0.000000	0.000000	0.259870
7	0.000000	1.381529	-0.106144
1	-0.293715	1.992551	0.652059
1	0.921981	1.662209	-0.428790
7	1.196439	-0.690765	-0.106144
1	1.872457	-0.741910	0.652059
1	0.978525	-1.629563	-0.428790
7	-1.196439	-0.690765	-0.106144
1	-1.578742	-1.250640	0.652059
1	-1.900506	-0.032646	-0.428790

**(CN, BH<sub>2</sub>, CH<sub>3</sub>)**

6	0.000000	0.410238	0.000000
5	1.193368	1.388949	0.000000
1	0.972728	2.563239	0.000000
1	2.311392	0.975523	0.000000
6	-1.444910	0.830709	0.000000
1	-1.971435	0.431756	0.878378
1	-1.971435	0.431756	-0.878378
1	-1.534633	1.919011	0.000000
6	0.256905	-0.972950	0.000000
7	0.479225	-2.124858	0.000000

**(CN, CN, CN)**

6	0.000000	0.000000	0.000000
6	0.000000	1.411538	0.000000
7	0.000000	2.580085	0.000000
6	1.222428	-0.705769	0.000000
7	2.234419	-1.290043	0.000000
6	-1.222428	-0.705769	0.000000
7	-2.234419	-1.290043	0.000000

**(F, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000000	0.000000	-0.066940
9	0.000000	0.000000	1.283873
5	0.000000	1.399437	-0.723514
1	0.000000	1.471920	-1.913551
1	0.000000	2.381008	-0.045485
5	0.000000	-1.399437	-0.723514
1	0.000000	-2.381008	-0.045485
1	0.000000	-1.471920	-1.913551

**(F, BH<sub>2</sub>, CN)**

6	0.000000	0.425433	0.000000
5	1.162513	1.416500	0.000000
1	0.922317	2.582149	0.000000
1	2.272488	0.988766	0.000000
9	-1.268091	0.856853	0.000000
6	0.111358	-0.983493	0.000000
7	0.248186	-2.145248	0.000000

**(F, BH<sub>2</sub>, F)**

6	0.000000	0.000000	0.065866
9	0.000000	1.077061	-0.695692
5	0.000000	0.000000	1.572086
1	0.000000	-1.048671	2.133412
1	0.000000	1.048671	2.133412
9	0.000000	-1.077061	-0.695692

**(F, F, F)**

6	0.000000	0.000000	0.328869
9	0.000000	1.264550	-0.073082
9	1.095133	-0.632275	-0.073082
9	-1.095133	-0.632275	-0.073082

**(NH<sub>2</sub>, BH<sub>2</sub>, CH<sub>3</sub>)**

6	0.000000	0.114105	0.000000
5	-0.241767	1.604112	0.000000
1	0.699029	2.354054	0.000000
1	-1.358713	2.034509	0.000000
7	1.269041	-0.382658	0.000000
1	1.469226	-1.373297	0.000000
1	2.057472	0.248362	0.000000
6	-1.077258	-0.938494	0.000000
1	-1.005370	-1.590332	0.883816
1	-1.005370	-1.590332	-0.883816
1	-2.067184	-0.478586	0.000000

**(NH<sub>2</sub>, BH<sub>2</sub>, CN)**

6	0.000000	0.421148	0.000000
5	-1.160560	1.401086	0.000000
1	-0.911058	2.573569	0.000000
1	-2.283539	1.005751	0.000000
6	-0.195234	-0.988787	0.000000
7	-0.362106	-2.144120	0.000000
7	1.302394	0.832046	0.000000
1	1.508347	1.820774	0.000000
1	2.078443	0.184828	0.000000

**(NH<sub>2</sub>, BH<sub>2</sub>, F)**

6	0.092165	-0.012806	-0.001863
9	-0.355656	1.258815	0.001386
7	-0.955036	-0.875026	-0.037838
1	-0.774225	-1.861143	0.077252
1	-1.891972	-0.539482	0.140958
5	1.554814	-0.349069	0.005210
1	1.860759	-1.506918	0.014191
1	2.364530	0.525570	0.005119

**(NH<sub>2</sub>, F, CH<sub>3</sub>)**

6	0.032602	0.013462	-0.286152
6	-1.377594	-0.366814	0.039659
1	-2.071087	0.348188	-0.412812
1	-1.557079	-0.378043	1.127538
1	-1.611056	-1.362777	-0.352411
9	0.330550	1.307263	0.052828
7	1.062633	-0.847631	0.141073
1	0.918908	-1.798922	-0.184151
1	1.976887	-0.520283	-0.162165

**(NH<sub>2</sub>, F, CN)**

6	-0.341441	-0.026659	0.048320
9	-0.955150	-1.220447	-0.018254
7	-1.186445	1.053605	-0.090676
1	-2.054718	0.978665	0.432624
1	-0.737622	1.954571	0.024908
6	1.039429	0.027478	0.002542
7	2.215126	0.095805	0.005188

**(CCH, CCH, CCH)**

6	0.000000	0.000000	0.000000
6	0.000000	1.408825	0.000000
6	0.000000	2.624889	0.000000
1	0.000000	3.691285	0.000000
6	1.220078	-0.704412	0.000000
6	2.273221	-1.312445	0.000000
1	3.196746	-1.845642	0.000000
6	-1.220078	-0.704412	0.000000
6	-2.273221	-1.312445	0.000000
1	-3.196746	-1.845642	0.000000

**(CCH, CCH, CN)**

6	0.000000	0.000000	0.011045
6	0.000000	0.000000	1.433306

7	0.000000	0.000000	2.600675
6	0.000000	1.224816	-0.672495
6	0.000000	2.285295	-1.268809
1	0.000000	3.217704	-1.787590
6	0.000000	-1.224816	-0.672495
6	0.000000	-2.285295	-1.268809
1	0.000000	-3.217704	-1.787590

**(CH<sub>3</sub>, CH<sub>3</sub>, CH<sub>3</sub>)**

6	0.000000	1.489244	-0.014637
6	0.000000	0.000000	0.143894
1	-0.888613	1.946601	0.439070
1	0.888613	1.946601	0.439070
1	0.000000	1.796405	-1.078107
6	1.289723	-0.744622	-0.014637
6	-1.289723	-0.744622	-0.014637
1	1.241500	-1.742862	0.439070
1	1.555732	-0.898202	-1.078107
1	2.130113	-0.203739	0.439070
1	-1.555732	-0.898202	-1.078107
1	-1.241500	-1.742862	0.439070
1	-2.130113	-0.203739	0.439070

**(CHO, CCH, CN)**

6	0.000000	0.136024	0.000000
6	1.453030	-0.144012	0.000000
8	1.915623	-1.268993	0.000000
1	2.089235	0.761338	0.000000
6	-0.911823	-0.946868	0.000000
7	-1.669633	-1.834758	0.000000
6	-0.464394	1.446972	0.000000
6	-0.835857	2.609713	0.000000
1	-1.172520	3.622944	0.000000

**(CHO, CHO, CHO)**

6	0.000000	0.000000	0.000000
6	0.000000	1.466854	0.000000
8	-1.039609	2.117672	0.000000
1	0.990154	1.951803	0.000000
6	-1.270333	-0.733427	0.000000
8	-1.314154	-1.959164	0.000000
1	-2.185388	-0.118403	0.000000
6	1.270333	-0.733427	0.000000
8	2.353762	-0.158508	0.000000
1	1.195234	-1.833400	0.000000

**(CHO, CHO, CN)**

6	0.000000	0.144079	0.000000
6	-0.953944	1.265657	0.000000
8	-2.162297	1.083957	0.000000
1	-0.516442	2.280548	0.000000
6	-0.486149	-1.251163	0.000000
8	0.267423	-2.209810	0.000000
1	-1.583176	-1.354303	0.000000
6	1.377513	0.408115	0.000000
7	2.519157	0.668637	0.000000

**(Cl, Cl, Cl)**

6	0.000000	0.000000	0.274604
17	0.000000	1.703168	-0.032306
17	-1.474987	-0.851584	-0.032306
17	1.474987	-0.851584	-0.032306

**(F, CHO, CCH)**

6	-0.058959	0.451333	-0.000006
6	1.158049	-0.214124	-0.000049
6	2.228104	-0.796217	0.000069
1	3.157326	-1.321191	-0.000001
6	-1.366734	-0.166635	0.000093
8	-1.541354	-1.380316	-0.000076
1	-2.203850	0.558903	0.000349
9	-0.042823	1.795408	-0.000041

**(NH<sub>2</sub>, CCH, CCH)**

6	0.006417	0.332548	0.000000
6	-0.018469	-0.353431	1.221392
6	-0.018469	-0.940381	2.288947
1	-0.046092	-1.465213	3.216294
6	-0.018469	-0.353431	-1.221392
6	-0.018469	-0.940381	-2.288947
1	-0.046092	-1.465213	-3.216294
7	-0.025301	1.733900	0.000000
1	0.337021	2.161793	0.844147
1	0.337021	2.161793	-0.844147

**(NH<sub>2</sub>, CCH, NH<sub>2</sub>)**

6	0.363136	0.000202	-0.002221
6	-1.016529	0.000015	0.002116
6	-2.235523	-0.000269	-0.002951
1	-3.292241	-0.000009	0.011244
7	1.135235	-1.170062	-0.075648
1	1.789396	-1.229104	0.681797

1	0.576697	-1.996991	-0.108940
7	1.133725	1.170703	0.076807
1	1.801464	1.223651	-0.668970
1	0.575462	1.998273	0.095088

**(NH<sub>2</sub>, CHO, CCH)**

6	0.043928	0.181577	-0.017114
6	1.409208	-0.137639	-0.006961
6	2.593570	-0.414580	0.012802
1	3.631228	-0.659585	0.026106
7	-0.388415	1.478504	-0.059872
1	-1.386052	1.586104	0.099514
1	0.220588	2.222919	0.249290
6	-0.985588	-0.836790	-0.005888
8	-2.185162	-0.546368	0.020307
1	-0.632274	-1.883432	-0.015301

**(NH<sub>2</sub>, CHO, NH<sub>2</sub>)**

6	0.408236	-0.015452	-0.004249
7	0.431838	1.356875	-0.086003
1	-0.513436	1.725613	-0.005261
1	1.104841	1.828277	0.509343
6	-0.846193	-0.680472	-0.016341
8	-1.930099	-0.052506	0.018883
1	-0.815300	-1.786759	-0.067284
7	1.621482	-0.671366	0.089057
1	1.555837	-1.679496	0.005255
1	2.363349	-0.290614	-0.490963

**(NH<sub>2</sub>, CN, CN)**

6	0.006420	0.309094	0.000000
7	-0.035670	1.689475	0.000000
1	0.223471	2.163772	0.855287
1	0.223471	2.163772	-0.855287
6	-0.009068	-0.390087	1.222457
7	-0.009068	-0.951957	2.248079
6	-0.009068	-0.390087	-1.222457
7	-0.009068	-0.951957	-2.248079

**(NH<sub>2</sub>, F, OH)**

6	0.019971	-0.003864	0.302539
9	0.315665	1.286270	-0.070480
7	-1.266919	-0.360278	-0.128590
1	-1.508116	-1.300435	0.167694
1	-1.963024	0.303522	0.194593
8	0.949123	-0.916347	-0.120549

1	1.785778	-0.703607	0.321317
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**(OH, OH, OH)**

6	0.001099	-0.014982	-0.323288
8	-1.122974	-0.727787	-0.016230
1	-1.553823	-0.323350	0.765248
8	-0.127780	1.299628	0.047864
1	0.758910	1.691536	0.034331
8	1.202533	-0.544229	0.117553
1	1.174088	-1.499193	-0.053349

**(CH=CH<sub>2</sub>, CH=CH<sub>2</sub>, CH=CH<sub>2</sub>)**

6	-0.168957	-0.230847	-0.013536
6	-1.517465	-0.730953	0.031318
6	-2.672614	-0.015038	0.011589
1	-1.608051	-1.815615	0.094163
1	-3.634654	-0.516904	0.034221
1	-2.694267	1.069827	-0.018381
6	0.060387	1.192579	-0.203882
6	1.117351	1.920954	0.209852
1	-0.741397	1.727263	-0.712090
1	1.165367	2.987538	0.010219
1	1.932107	1.495586	0.786020
6	0.886934	-1.201700	0.110030
6	2.211119	-1.056020	-0.153451
1	0.554715	-2.194427	0.416407
1	2.890394	-1.893813	-0.029493
1	2.635255	-0.133302	-0.532577

**(NH<sub>2</sub>, BH<sub>2</sub>, CCH)**

6	0.447102	0.060306	0.000000
6	-0.967798	0.059279	0.000001
6	-2.182984	0.054944	-0.000001
1	-3.248952	0.079431	0.000003
7	1.048556	-1.170704	-0.000004
1	2.055836	-1.232154	0.000012
1	0.516976	-2.029040	0.000014
5	1.270525	1.336163	0.000000
1	0.737365	2.402869	0.000003
1	2.468337	1.245834	0.000000

**(NH<sub>2</sub>, CHO, BH<sub>2</sub>)**

6	0.000000	0.510319	0.000000
6	-0.740178	-0.759826	0.000000
8	-0.182859	-1.853942	0.000000
1	-1.841550	-0.672248	0.000000

7	1.340943	0.338020	0.000000
1	1.979348	1.119670	0.000000
1	1.702726	-0.611411	0.000000
5	-0.682971	1.866835	0.000000
1	-0.031773	2.872385	0.000000
1	-1.876557	1.919876	0.000000

**(NH<sub>2</sub>, CHO, CF<sub>3</sub>)**

6	0.518077	0.231531	-0.029452
6	1.570257	-0.741939	-0.012500
8	2.760382	-0.394790	0.008606
1	1.272579	-1.802720	-0.027254
7	0.856094	1.540525	0.049106
1	0.200368	2.260639	-0.217873
1	1.851062	1.729608	-0.020709
6	-0.934091	-0.118015	-0.001885
9	-1.438288	-0.146035	1.253129
9	-1.661965	0.800688	-0.689282
9	-1.158100	-1.326024	-0.550929

**(NH<sub>2</sub>, CHO, CH<sub>3</sub>)**

6	-0.387456	0.016069	0.003021
6	0.840790	-0.710398	0.002621
8	1.952191	-0.144599	-0.012593
1	0.755071	-1.813467	0.014370
7	-0.285714	1.371834	0.055244
1	0.658069	1.729110	-0.057276
1	-1.053394	1.963742	-0.226253
6	-1.735638	-0.626994	-0.004747
1	-2.329926	-0.318263	-0.877151
1	-2.315175	-0.362941	0.890813
1	-1.638355	-1.716289	-0.035838

**(NH<sub>2</sub>, CHO, CH=CH<sub>2</sub>)**

6	-0.030151	0.338911	-0.019511
6	-0.811196	-0.878029	-0.037924
8	-2.047148	-0.865599	0.025083
1	-0.256199	-1.828228	-0.121486
7	-0.768714	1.491214	-0.029060
1	-1.762610	1.350927	0.118861
1	-0.367851	2.355192	0.305850
6	1.403630	0.398203	-0.045541
6	2.274565	-0.636525	0.048751
1	1.821898	1.400732	-0.148376
1	3.343975	-0.460158	0.004690
1	1.957887	-1.667539	0.168575



**(NH<sub>2</sub>, CHO, CHO)**

6	0.000000	0.000000	0.004567
6	0.000000	1.275526	-0.684482
8	0.000000	2.349495	-0.084222
1	0.000000	1.226938	-1.790129
6	0.000000	-1.275526	-0.684482
8	0.000000	-2.349495	-0.084222
1	0.000000	-1.226938	-1.790129
7	0.000000	0.000000	1.347916
1	0.000000	-0.884369	1.839385
1	0.000000	0.884369	1.839385

**(NH<sub>2</sub>, CHO, CN)**

6	0.072639	0.177150	-0.005991
6	-0.974420	-0.828185	-0.004266
8	-2.162563	-0.504454	0.010987
1	-0.644922	-1.880558	-0.014776
7	-0.321738	1.475849	-0.030671
1	-1.321119	1.630871	0.047282
1	0.320324	2.238878	0.118053
6	1.440507	-0.168605	-0.002488
7	2.566576	-0.480952	0.007531

**(NH<sub>2</sub>, CHO, F)**

6	0.404265	-0.053932	-0.002354
6	-0.882884	-0.634424	-0.005005
8	-1.905980	0.086044	0.018447
1	-0.919394	-1.736410	-0.026650
7	0.609392	1.283056	-0.072861
1	-0.242468	1.820048	0.052101
1	1.460122	1.665460	0.318936
9	1.506173	-0.809855	0.006914

**(NH<sub>2</sub>, CHO, OH)**

6	0.421604	-0.011051	-0.003850
6	-0.793531	-0.735561	-0.000597
8	-1.875350	-0.082284	0.008272
1	-0.764433	-1.836076	-0.003317
7	1.683999	-0.523045	-0.066418
1	2.432709	0.086090	0.238261
1	1.796211	-1.496030	0.184250
8	0.329288	1.322919	0.000623
1	-0.652425	1.461924	0.001250

**(NH<sub>2</sub>, BH<sub>2</sub>, CH=CH<sub>2</sub>)**

6	-0.527918	-0.050833	0.008825
7	-0.608832	1.314589	-0.014100
1	0.181458	1.897877	0.223572
1	-1.518627	1.746477	0.054383
5	-1.797483	-0.885372	-0.029349
1	-1.729540	-2.079070	-0.013569
1	-2.867707	-0.341882	-0.072402
6	0.780753	-0.668384	0.042529
6	1.983797	-0.054555	-0.037335
1	0.758678	-1.751348	0.134144
1	2.906882	-0.623850	0.005187
1	2.098303	1.019160	-0.169980

**(NH<sub>2</sub>, BH<sub>2</sub>, OH)**

6	0.062158	-0.034653	-0.004035
7	-1.112729	-0.716759	-0.043297
1	-1.979102	-0.231459	0.147879
1	-1.091533	-1.713522	0.105832
5	1.437301	-0.651371	0.005225
1	2.388244	0.081624	0.007334
1	1.559091	-1.841909	0.012597
8	-0.168267	1.305783	0.003098
1	0.699087	1.741089	0.002732

**(OH, BH<sub>2</sub>, BH<sub>2</sub>)**

6	0.000000	0.065120	0.000000
8	-0.409019	-1.228893	0.000000
1	0.374524	-1.811786	0.000000
5	-1.139319	1.108394	0.000000
1	-2.281702	0.758436	0.000000
1	-0.858439	2.268502	0.000000
5	1.507416	0.355882	0.000000
1	2.277656	-0.569788	0.000000
1	1.919622	1.473689	0.000000

**(OH, BH<sub>2</sub>, CCH)**

6	0.000000	0.438309	0.000000
8	-1.279881	0.903287	0.000000
1	-1.232192	1.875319	0.000000
5	1.199651	1.370023	0.000000
1	0.993383	2.553971	0.000000
1	2.310346	0.940143	0.000000
6	0.093337	-0.964795	0.000000
6	0.214211	-2.175135	0.000000
1	0.323967	-3.236115	0.000000

**(OH, BH<sub>2</sub>, OH)**

6	0.000000	0.086483	0.000000
8	1.318357	-0.145597	0.000000
1	1.467820	-1.109261	0.000000
5	-0.619025	1.459680	0.000000
1	0.068604	2.431714	0.000000
1	-1.817369	1.519963	0.000000
8	-0.691435	-1.078778	0.000000
1	-1.639308	-0.864713	0.000000

**(OH, CHO, CCH)**

6	0.000000	0.191249	0.000000
8	-0.784822	1.279791	0.000000
1	-1.699512	0.904759	0.000000
6	1.388817	0.331806	0.000000
6	2.603128	0.403651	0.000000
1	3.667720	0.473540	0.000000
6	-0.688889	-1.078227	0.000000
8	-1.927816	-1.088626	0.000000
1	-0.085430	-1.998496	0.000000

**(OH, CHO, CHO)**

6	0.000000	0.027876	0.000000
8	-1.104004	0.760924	0.000000
1	-1.843863	0.105333	0.000000
6	1.302343	0.675589	0.000000
8	1.468887	1.886534	0.000000
1	2.156705	-0.032247	0.000000
6	-0.184982	-1.409305	0.000000
8	-1.330576	-1.870425	0.000000
1	0.708538	-2.054310	0.000000

**(OH, CHO, OH)**

6	0.000000	0.427229	0.000000
8	1.324659	0.273066	0.000000
1	1.425013	-0.713130	0.000000
6	-0.810459	-0.727415	0.000000
8	-0.227071	-1.846347	0.000000
1	-1.901929	-0.612467	0.000000
8	-0.466296	1.677746	0.000000
1	0.289330	2.290994	0.000000

**(NH<sub>2</sub>, BH<sub>2</sub>, COOH)**

6	0.008374	-0.745452	0.000000
6	0.000000	0.734532	0.000000
8	-1.024309	1.404057	0.000000

7	-1.257395	-1.235610	0.000000
1	-1.427175	-2.230347	0.000000
1	-2.037415	-0.587047	0.000000
5	1.224607	-1.651458	0.000000
1	1.044169	-2.838182	0.000000
1	2.329796	-1.210309	0.000000
8	1.229294	1.293563	0.000000
1	1.079229	2.257001	0.000000

**(NH<sub>2</sub>, CHO, COOH)**

6	0.000000	0.359745	0.000000
6	1.431395	0.571597	0.000000
8	1.909762	1.709376	0.000000
1	2.065045	-0.329523	0.000000
6	-0.678784	-0.934540	0.000000
8	-1.894051	-1.058156	0.000000
7	-0.793964	1.449391	0.000000
1	-1.798574	1.342158	0.000000
1	-0.349117	2.358601	0.000000
8	0.173459	-1.990100	0.000000
1	-0.388637	-2.786741	0.000000

**(SH, NH<sub>2</sub>, NH<sub>2</sub>)**

7	-1.222307	-1.125948	-0.027922
1	-0.805420	-1.981748	-0.378850
1	-1.534159	-1.264547	0.938875
6	-0.418867	0.003355	-0.244699
16	1.346496	-0.087435	0.093191
1	1.748544	0.766103	-0.876773
7	-1.023305	1.251616	-0.032550
1	-2.036914	1.193645	-0.047117
1	-0.683500	1.785698	0.764303

**(SH, SH, NH<sub>2</sub>)**

7	-0.028454	1.692248	0.097935
1	0.864327	2.158911	-0.019496
1	-0.790651	2.201192	-0.342471
6	0.005703	0.327949	-0.206179
16	-1.556900	-0.485250	0.084068
1	-1.396706	-1.453112	-0.843235
16	1.550528	-0.512233	-0.054828
1	1.589940	-0.760694	1.288882

**(SH, SH, SH)**

6	-0.000485	-0.007732	-0.097436
16	1.531773	-0.870934	-0.062430

1	2.072008	-0.298361	1.044744
16	-1.465351	-0.970334	0.060601
1	-2.267436	-0.197069	-0.709526
16	-0.109366	1.746486	0.067203
1	0.885429	2.058342	-0.796582

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, BH<sub>2</sub>)**

6	-0.532873	0.012448	0.000622
5	-0.690283	1.546032	0.040339
1	0.074581	2.249735	0.639092
1	-1.619968	2.063949	-0.506465
6	0.730683	-0.643638	0.008159
6	1.958926	-0.028153	-0.056679
1	0.726423	-1.734647	0.038099
1	2.878548	-0.605989	-0.057453
1	2.054228	1.053102	-0.089103
5	-1.801702	-0.870862	0.005990
1	-2.868991	-0.419860	-0.290897
1	-1.725313	-2.026072	0.322475

**(CH=CH<sub>2</sub>, BH<sub>2</sub>, CH=CH<sub>2</sub>)**

6	0.000000	0.000000	0.115792
6	0.000000	1.220532	-0.654625
6	0.000000	2.495060	-0.182685
1	0.000000	1.100818	-1.740809
1	0.000000	3.338338	-0.866649
1	0.000000	2.720802	0.878132
5	0.000000	0.000000	1.652549
1	0.000000	-1.020888	2.274435
1	0.000000	1.020888	2.274435
6	0.000000	-1.220532	-0.654625
6	0.000000	-2.495060	-0.182685
1	0.000000	-1.100818	-1.740809
1	0.000000	-3.338338	-0.866649
1	0.000000	-2.720802	0.878132

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