Table S1 Intramolecular triel bond energy, $-E_{int}$ (kcal/mol)

			B···S	B···O	Al···O	Ga···O	In···O
H	H	H	48.89	52.53	19.34	27.41	16.74
NO_2	H	H	63.34	84.15	24.85	34.10	20.72
H	NO_2	H	65.61	77.98	20.36	28.43	16.38
H	H	NO_2	65.87	85.18	22.35	31.09	17.41
CH_3	H	H	62.68	80.84	23.25	32.23	19.52
H	CH_3	H	62.80	83.86	26.05	35.57	22.02
H	H	CH_3	63.07	85.42	26.84	36.14	22.25
NO_2	CH_3	H	63.34	83.52	24.49	33.70	20.51
NO_2	H	CH_3	63.82	83.41	25.33	34.75	21.14
CH_3	NO_2	H	64.00	84.69	25.82	35.03	21.48
CH_3	H	NO_2	63.82	83.41	25.34	34.75	21.14
H	NO_2	CH_3	63.00	79.01	22.53	30.63	18.02
H	CH_3	NO_2	66.99	86.80	25.60	35.39	21.26

Table S2 Laplacian ($\nabla^2\rho$), kinetic energy density (G) and total energy density (H) at the Tr···S BCP, all in a.u.

			$\nabla^2\rho$			G			H		
R_1	R_2	R_3	Al···S	Ga···S	In···S	Al···S	Ga···S	In···S	Al···S	Ga···S	In···S
	alkyl		0.1264	0.1184	0.1079	0.0353	0.0417	0.0333	-0.0037	-0.0121	-0.0063
H	H	H	0.1469	0.1328	0.1217	0.0422	0.0505	0.0397	-0.0055	-0.0174	-0.0093
NO_2	H	H	0.1335	0.1270	0.1106	0.0377	0.0467	0.0347	-0.0044	-0.0149	-0.0071
H	NO_2	H	0.1418	0.1282	0.1176	0.0407	0.0484	0.0381	-0.0052	-0.0163	-0.0087
H	H	NO_2	0.1357	0.1357	0.1283	0.0383	0.0468	0.0362	-0.0043	-0.0043	-0.0147
CH_3	H	H	0.1550	0.1351	0.1263	0.0450	0.0525	0.0420	-0.0063	-0.0187	-0.0104
H	CH_3	H	0.1480	0.1334	0.1227	0.0424	0.0505	0.0399	-0.0054	-0.0172	-0.0092
H	H	CH_3	0.1520	0.1353	0.1251	0.0438	0.0518	0.0411	-0.0058	-0.018	-0.0098
NO_2	CH_3	H	0.1523	0.1364	0.1245	0.0438	0.0526	0.0409	-0.0058	-0.0185	-0.0098
NO_2	H	CH_3	0.1390	0.1295	0.1142	0.0395	0.0481	0.0362	-0.0047	-0.0158	-0.0077
CH_3	NO_2	H	0.1521	0.1339	0.1244	0.0441	0.0517	0.0410	-0.0060	-0.0183	-0.0099
CH_3	H	NO_2	0.1443	0.1314	0.1203	0.0411	0.0491	0.0385	-0.0050	-0.0163	-0.0085
H	NO_2	CH_3	0.1496	0.2587	0.1231	0.0429	0.1024	0.0410	-0.0055	-0.0027	-0.0093
H	CH_3	NO_2	0.1497	0.1344	0.1296	0.0429	0.0510	0.0425	-0.0055	-0.0175	-0.0101

Table S3 Binding distance (R, Å), interaction energy (E_{int}, kcal/mol), electron density (ρ), Laplacian ($\nabla^2\rho$, a.u.), kinetic energy density (G, a.u.) and potential energy density (V, a.u.) at the Tr···S BCP in complexes between SCHR (R=H, CH_3, NO_2) and TrH_2CRCHR (Tr= Al, Ga, In; R=H, CH_3, NO_2)

	R	E_{int}	ρ	$\nabla^2\rho$	G	V
AlH_2CHCH_2···SCHH	2.554	-18.99	0.0305	0.1109	0.0302	-0.0328
AlH_2CHCH_2···$SCHNO_2$	2.605	-17.46	0.0260	0.0949	0.0253	-0.0268
AlH_2CHCH_2···$SCHCH_3$	2.544	-19.72	0.0314	0.1136	0.0312	-0.0340
$AlH_2CNO_2CH_2$···SCHH	2.518	-20.51	0.0337	0.1215	0.0338	-0.0372
$AlH_2CNO_2CH_2$···$SCHNO_2$	2.569	-18.45	0.0288	0.1038	0.0281	-0.0303
$AlH_2CNO_2CH_2$···$SCHCH_3$	2.503	-21.20	0.0351	0.1261	0.0354	-0.0393
$AlH_2CCH_3CH_2$···SCHH	2.558	-18.85	0.0304	0.1095	0.0300	-0.0325
$AlH_2CCH_3CH_2$···$SCHNO_2$	2.609	-17.33	0.0259	0.0937	0.0250	-0.0266
$AlH_2CCH_3CH_2$···$SCHCH_3$	2.545	-19.69	0.0314	0.1128	0.0311	-0.0340
$AlH_2CHCHNO_2$···SCHH	2.528	-20.02	0.0327	0.1196	0.0329	-0.0359
$AlH_2CHCHNO_2$···$SCHNO_2$	2.572	-18.32	0.0283	0.1050	0.0281	-0.0300
$AlH_2CHCHNO_2$···$SCHCH_3$	2.516	-20.87	0.0339	0.1230	0.0342	-0.0376
$AlH_2CHCHCH_3$···SCHH	2.558	-18.77	0.0301	0.1096	0.0299	-0.0323
$AlH_2CHCHCH_3$···$SCHNO_2$	2.611	-17.25	0.0256	0.0932	0.0248	-0.0263
$AlH_2CHCHCH_3$···$SCHCH_3$	2.547	-19.37	0.0311	0.1123	0.0308	-0.0336
$AlH_2CNO_2CHCH_3$···SCHH	2.518	-20.66	0.0338	0.1218	0.0339	-0.0374
$AlH_2CNO_2CHCH_3$···$SCHNO_2$	2.571	-18.47	0.0284	0.1037	0.0281	-0.0303
$AlH_2CNO_2CHCH_3$···$SCHCH_3$	2.503	-21.15	0.0352	0.1260	0.0354	-0.0393
$AlH_2CCH_3CHNO_2$···SCHH	2.538	-19.95	0.0321	0.1157	0.0320	-0.0350
$AlH_2CCH_3CHNO_2$··$SCHNO_2$	2.582	-18.27	0.0277	0.1014	0.0274	-0.0297

	3	18.11	7	1	2	0.0291
$AlH_2CCH_3CHNO_2\cdots SCHCH_3$	2.52	-	0.033	0.119	0.033	-
	4	20.26	4	6	3	0.0367
$GaH_2CHCH_2\cdots SCHH$	2.63	-	0.037	0.092	0.029	-
	4	16.89	2	6	6	0.0361
$GaH_2CHCH_2\cdots SCHNO_2$	2.73	-	0.029	0.079	0.022	-
	0	14.23	2	0	9	0.0261
$GaH_2CHCH_2\cdots SCHCH_3$	2.61	-	0.038	0.094	0.030	-
	6	17.74	8	8	9	0.0382
$GaH_2CNO_2CH_2\cdots SCHH$	2.58	-	0.042	0.099	0.033	-
	3	19.26	2	9	8	0.0427
$GaH_2CNO_2CH_2\cdots SCHNO_2$	2.67	-	0.033	0.086	0.026	-
	3	15.59	6	2	6	0.0316
$GaH_2CNO_2CH_2\cdots SCHCH_3$	2.53	-	0.047	0.107	0.038	-
	4	20.77	3	9	3	0.0496
$GaH_2CCH_3CH_2\cdots SCHH$	2.63	-		0.091	0.029	-
	8	16.62	0.037	8	4	0.0358
$GaH_2CCH_3CH_2\cdots SCHNO_2$	2.73	-	0.029	0.078	0.022	-
	2	14.12	1	6	8	0.0260
$GaH_2CCH_3CH_2\cdots SCHCH_3$	2.62	-	0.038	0.093	0.030	-
	1	17.46	5	7	5	0.0377
$GaH_2CHCHNO_2\cdots SCHH$	2.59	-	0.041	0.099	0.033	-
	3	18.47	1	5	1	0.0413
$GaH_2CHCHNO_2\cdots SCHNO_2$	2.67	-	0.033	0.087	0.026	-
	5	15.47	1	4	6	0.0313
$GaH_2CHCHNO_2\cdots SCHCH_3$	2.57	-	0.042	0.099	0.033	-
	3	19.26	3	8	8	0.0427
$GaH_2CHCHCH_3\cdots SCHH$	2.64	-	0.036	0.091	0.028	-
	4	16.64	4	1	9	0.0350
$GaH_2CHCHCH_3\cdots SCHNO_2$	2.75	-	0.027	0.076	0.021	-
	0	13.65	9	1	8	0.0246
$GaH_2CHCHCH_3\cdots SCHCH_3$	2.62	-	0.037	0.093	0.030	-
	6	17.06	9	2	1	0.0370
$GaH_2CNO_2CHCH_3\cdots SCHH$	2.58	-	0.042	0.099	0.033	-
	6	19.15	1	3	6	0.0424
$GaH_2CNO_2CHCH_3\cdots SCHNO_2$	2.69	-	0.032	0.081	0.024	-
	9	14.81	1	5	9	0.0294
$GaH_2CNO_2CHCH_3\cdots SCHCH_3$	2.56	-	0.044	0.102	0.035	-
	2	19.98	4	6	6	0.0455
$GaH_2CCH_3CHNO_2\cdots SCHH$	2.60	-	0.040	0.097	0.032	-
	4	18.16	2	0	1	0.0399
$GaH_2CCH_3CHNO_2\cdot\cdot SCHNO_2$	2.68	-	0.032	0.085	0.025	-
	8	15.01	3	0	6	0.0300
$GaH_2CCH_3CHNO_2\cdots SCHCH$	2.58	-	0.042	0.099	0.033	-

$_3$	3	19.22	3	8	8	0.0427
$InH_2CHCH_2\cdots SCHH$	2.89	-	0.029	0.077	0.021	-
	1	14.55	3	0	8	0.0243
$InH_2CHCH_2\cdots SCHNO_2$	3.03	-	0.021	0.059	0.015	-
	1	12.06	1	0	3	0.0158
$InH_2CHCH_2\cdots SCHCH_3$	2.86	-	0.031	0.081	0.023	-
	1	15.39	3	4	4	0.0265
$InH_2CNO_2CH_2\cdots SCHH$	2.82	-	0.033	0.086	0.025	-
	9	16.12	7	1	4	0.0293
$InH_2CNO_2CH_2\cdots SCHNO_2$	2.95	-	0.025	0.067	0.018	-
	4	13.04	0	7	3	0.0198
$InH_2CNO_2CH_2\cdots SCHCH_3$	2.79	-	0.036	0.091	0.027	-
	6	16.70	2	5	6	0.0322
$InH_2CCH_3CH_2\cdots SCHH$	2.89	-	0.029	0.077	0.021	-
	0	14.61	4	1	8	0.0244
$InH_2CCH_3CH_2\cdots SCHNO_2$	3.02	-	0.021	0.059	0.015	-
	7	12.21	4	3	4	0.0160
$InH_2CCH_3CH_2\cdots SCHCH_3$	2.85	-	0.031	0.081	0.023	-
	8	15.36	5	7	6	0.0267
$InH_2CHCHNO_2\cdots SCHH$	2.85	-	0.032	0.083	0.024	-
	1	15.77	2	2	2	0.0275
$InH_2CHCHNO_2\cdots SCHNO_2$	2.96	-	0.024	0.066	0.017	-
	7	12.91	3	9	9	0.0191
$InH_2CHCHNO_2\cdots SCHCH_3$	2.82	-	0.034	0.087	0.025	-
	1	16.46	3	6	9	0.0300
$InH_2CHCHCH_3\cdots SCHH$	2.89	-	0.028	0.076	0.021	-
	6	14.38	9	2	5	0.0239
$InH_2CHCHCH_3\cdots SCHNO_2$	3.04	-	0.020	0.057	0.014	-
	3	11.88	6	6	8	0.0152
$InH_2CHCHCH_3\cdots SCHCH_3$	2.86	-	0.030	0.080	0.023	-
	5	15.01	9	7	2	0.0261
$InH_2CNO_2CHCH_3\cdots SCHH$	2.82	-	0.034	0.086	0.025	-
	6	16.22	0	6	6	0.0296
$InH_2CNO_2CHCH_3\cdots SCHNO_2$	2.93	-	0.025	0.070	0.019	-
	9	13.33	9	0	1	0.0207
$InH_2CNO_2CHCH_3\cdots SCHCH_3$	2.79	-	0.036	0.091	0.027	-
	4	16.98	4	7	7	0.0324
$InH_2CCH_3CHNO_2\cdots SCHH$	2.85	-	0.031	0.081	0.023	-
	8	15.49	7	8	7	0.0269
$InH_2CCH_3CHNO_2\cdot SCHNO_2$	2.97	-	0.023	0.065	0.017	-
	7	12.72	9	4	5	0.0186
$InH_2CCH_3CHNO_2\cdots SCHCH_3$	2.82	-	0.033	0.086	0.025	-
	8	16.15	9	2	5	0.0294

Table S4 Triel bond energy, $-E_{int}$ (kcal/mol) of intramolecular TrBs within the five-membered rings and the corresponding intermolecular binary systems.

			intra			inter		
R_1	R_2	R_3	Al···S	Ga···S	In···S	Al···S	Ga···S	In···S
H	H	H	14.37	20.45	14.73	18.99	16.89	14.55
NO_2	H	H	12.68	18.55	12.59	17.46	19.26	16.12
H	NO_2	H	13.83	19.49	14.10	20.02	18.47	15.77
H	H	NO_2	12.83	18.52	13.13	17.46	14.23	12.06
CH_3	H	H	15.45	21.48	15.75	18.85	16.62	14.61
H	CH_3	H	14.37	20.39	14.82	18.77	16.64	14.38
H	H	CH_3	14.91	21.05	15.33	19.72	17.74	15.39
NO_2	CH_3	H	14.94	21.39	15.27	20.66	19.15	16.22
NO_2	H	CH_3	13.31	19.25	13.22	21.20	20.77	16.70
CH_3	NO_2	H	15.09	21.05	15.33	19.95	18.16	15.49
CH_3	H	NO_2	13.92	19.67	14.13	17.33	14.12	12.21
H	NO_2	CH_3	14.55	20.63	14.85	20.87	19.26	16.46
H	CH_3	NO_2	14.58	20.63	15.87	17.25	13.65	11.88

Table S5 Natural charges (q, e) on the Tr, S and C_1 atoms

			q_{Tr}			q_S			q_{C1}		
R_1	R_2	R_3	Al···S	Ga···S	In···S	Al···S	Ga···S	In···S	Al···S	Ga···S	In···S
	alkyl		1.241	1.000	1.094	0.036	0.064	0.033	-0.934	-0.862	-0.849
H	H	H	1.179	0.933	1.058	-0.041	-0.035	-0.035	-0.413	-0.358	-0.369
NO_2	H	H	1.179	0.932	1.057	-0.034	-0.032	-0.029	-0.201	-0.147	-0.160
H	NO_2	H	1.179	0.932	1.057	-0.025	-0.025	-0.023	-0.351	-0.299	-0.309
H	H	NO_2	1.174	0.932	1.054	-0.088	-0.088	-0.084	-0.391	-0.339	-0.347
CH_3	H	H	1.191	0.938	1.069	-0.077	-0.067	-0.065	-0.180	-0.133	-0.137
H	CH_3	H	1.184	0.934	1.067	-0.048	-0.048	-0.041	-0.446	-0.389	-0.399
H	H	CH_3	1.189	0.935	1.068	-0.060	-0.053	-0.052	-0.422	-0.366	-0.377
NO_2	CH_3	H	1.224	0.952	1.127	-0.044	-0.044	-0.042	-0.141	-0.086	-0.094
NO_2	H	CH_3	1.190	0.935	1.075	-0.034	-0.034	-0.032	-0.203	-0.150	-0.162
CH_3	NO_2	H	1.204	0.975	1.107	-0.043	-0.041	-0.038	-0.137	-0.089	-0.100
CH_3	H	NO_2	1.189	0.935	1.067	-0.028	-0.027	-0.022	-0.158	-0.113	-0.116
H	NO_2	CH_3	1.200	0.947	1.084	-0.042	-0.033	-0.035	-0.382	-0.327	-0.343
H	CH_3	NO_2	1.204	0.952	1.088	-0.042	-0.033	-0.035	-0.382	-0.327	-0.343

Table S6 Multi-center bond order in natural atomic orbital (NAO) basis

R_1	R_2	R_3	Al···S	Ga···S	In···S
	alkyl		0.2628	0.2674	0.2714
H	H	H	0.3140	0.3331	0.3162
NO_2	H	H	0.3104	0.3313	0.3110
H	NO_2	H	0.3128	0.3324	0.3150
H	H	NO_2	0.3135	0.3329	0.3240
CH_3	H	H	0.3194	0.3370	0.3205
H	CH_3	H	0.3211	0.3402	0.3222
H	H	CH_3	0.3184	0.3340	0.3187
NO_2	CH_3	H	0.3158	0.3334	0.3125
NO_2	H	CH_3	0.3143	0.3217	0.3021
CH_3	NO_2	H	0.3163	0.3334	0.3173
CH_3	H	NO_2	0.3148	0.3350	0.3187
H	NO_2	CH_3	0.3109	0.3276	0.3116
H	CH_3	NO_2	0.3109	0.3276	0.3141

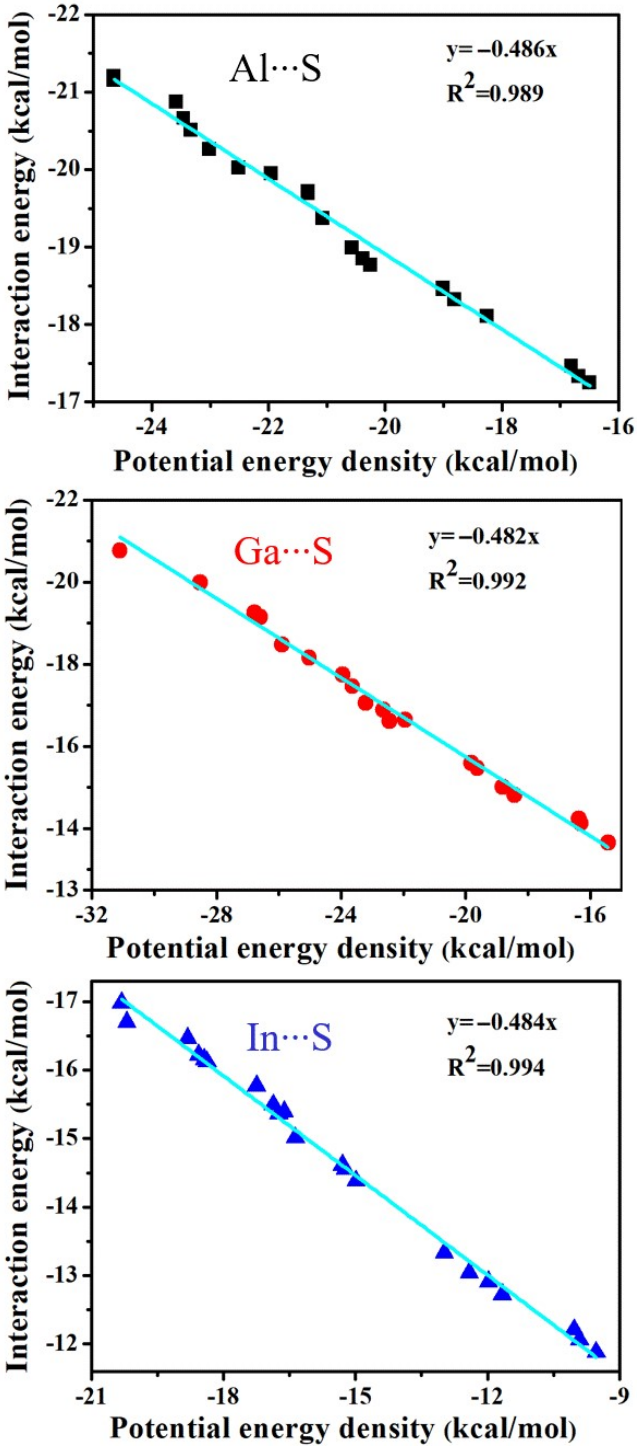

Figure S1 The linear relationship between the interaction energy (E_{int}, kcal/mol) and potential energy density (V, kcal/mol) in complexes between SCHX (X=H, CH_3, NO_2) and TrH_2CYCHY (Tr= Al, Ga, In; Y=H, CH_3, NO_2).

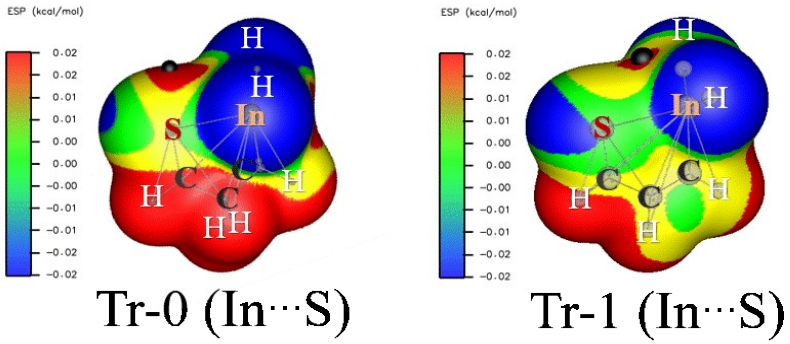

Figure S2 MEP maps of the five-membered closed system on the 0.001 electrons bohr^{-3} isosurface. Color ranges, in au, are: red, > 0.02; yellow, 0.02–0.01; green, 0.01 – -0.02; blue, < -0.02.

CARTESIAN COORDINATES

Al(Tr-0)

C	-0.95459200	1.26327800	-0.32779100
C	0.44653600	1.59091600	0.18486600
H	-1.66266500	1.99693700	0.06227900
H	-0.96360400	1.36737100	-1.41682700
C	1.41264400	0.46253800	0.06696500
H	0.90632400	2.46790500	-0.28325800
H	0.41939200	1.82615200	1.25965700
H	2.47462100	0.69415600	0.12639700
H	-2.16547600	-1.52618700	-0.96325000
H	-1.62710900	-0.97247900	1.67770200
S	0.99885500	-1.10316300	-0.10617900
Al	-1.44543800	-0.62335700	0.13014800

Al(Tr-1)

C	0.87149000	1.39034200	-0.00868500
C	-0.46974200	1.60999900	0.00036800
H	1.49373200	2.28226600	-0.01165000
C	-1.38342200	0.49214000	0.00521600
H	-0.92071200	2.59751500	0.00560400
H	-2.45025300	0.70179900	0.01743200
H	1.95079600	-1.07740900	1.40956400
H	2.01163400	-1.10088300	-1.36671000
S	-0.93642300	-1.09099900	-0.00540800
Al	1.44520100	-0.53093700	0.00391500

Al(Tr-2)

C	1.47668400	1.54205700	-0.21732700
C	0.12393900	1.41610800	-0.20070500
C	-0.43694400	0.10152400	-0.02690300
H	3.15207300	-0.36647300	1.47699300
H	3.16551200	-0.75837600	-1.28376900
H	1.84634500	2.55340400	-0.36897700
S	0.35639000	-1.31614900	0.16759900
H	-0.58221700	2.23048900	-0.31152300
N	-1.93146400	0.04622400	-0.01065300
O	-2.48483600	0.97707800	0.57289900
O	-2.47487800	-0.90585700	-0.55955300
Al	2.53322600	-0.14247100	0.03408500

Al(Tr-3)

C	-0.54882900	-0.13585700	-0.00417000
C	0.03512500	-1.35758700	0.00642500

C	1.47707400	-1.40242500	0.00546300
H	-0.53187100	-2.28135900	0.01612200
H	1.95869800	-2.37629300	0.01059600
H	0.71422700	2.23648000	1.40985700
H	0.71815400	2.25686400	-1.40267500
S	2.45469100	-0.07953700	-0.00253500
N	-2.00534700	-0.08876200	-0.00146800
O	-2.48235100	1.05657500	0.01193700
O	-2.66958000	-1.12675800	-0.01202800
Al	0.56449100	1.53807000	-0.00220400

Al(Tr-4)

C	0.06839400	-1.30851600	0.00014100
C	-0.58091200	-0.13213900	-0.00002700
C	0.10013200	1.14595700	-0.00014400
H	-0.50552000	2.04514500	-0.00020600
H	2.76294900	-1.44277500	-1.39675200
H	2.76271100	-1.44224800	1.39736600
H	-0.56883000	-2.18814600	0.00027600
N	-2.06990600	-0.05565600	-0.00000400
O	-2.57324900	1.06829900	0.00050500
O	-2.69110300	-1.11067500	-0.00045800
S	1.73024800	1.28330200	-0.00015700
Al	2.07255400	-1.15446200	0.00012800

Al(Tr-5)

C	0.91258800	1.54809000	-0.00081100
C	-0.43735500	1.41971800	-0.00056200
C	-1.06610500	0.11017300	-0.00015900
H	2.62647200	-0.55942800	1.38856600
H	2.63559500	-0.55884000	-1.38223200
H	1.28528400	2.57005000	-0.00177800
H	-1.12077400	2.26593800	-0.00054000
C	-2.56017300	0.06891900	0.00111700
H	-2.93210500	0.60298700	0.87824500
H	-2.93362400	0.60182500	-0.87603900
H	-2.94265700	-0.94701400	0.00213500
S	-0.19763800	-1.29575700	-0.00115000
Al	1.95771400	-0.16344700	0.00096400

Al(Tr-6)

C	1.20930800	-0.14796100	-0.00035800
C	0.53600300	-1.33337700	-0.00023600
C	-0.89642700	-1.36288300	0.00008300

H	-0.06434000	2.24977100	-1.38800700
H	-0.06319700	2.24940700	1.38873600
H	-1.38512200	-2.33449000	0.00024800
H	1.04402300	-2.29595800	-0.00029200
C	2.70290500	-0.15753600	-0.00030800
H	3.07971800	0.38231600	0.87167100
H	3.12729400	-1.16342900	-0.00075700
H	3.08016600	0.38378400	-0.87134000
S	-1.88654000	-0.04087200	0.00000500
Al	0.00425900	1.47639200	0.00035100

Al(Tr-7)

C	-0.47602000	-1.32340300	-0.00082000
C	-1.23144300	-0.18909800	-0.00006700
C	-0.54411300	1.08728200	0.00051400
H	2.24654500	-1.36803200	-1.38376100
H	2.24219800	-1.36465600	1.38764100
H	-1.04084000	-2.25473500	-0.00124100
S	1.08508800	1.30927800	-0.00048400
H	-1.15706200	1.98786400	0.00170000
C	-2.73677100	-0.13197200	0.00008200
H	-3.15643800	-1.13506700	0.00082600
H	-3.10634700	0.39733100	0.87968100
H	-3.10648900	0.39596100	-0.88023200
Al	1.51131600	-1.09722800	0.00037500

Al(Tr-8)

C	0.29886900	-1.51392100	0.05346700
C	-0.46333900	-0.40825800	0.00505900
C	0.06831800	0.95068500	-0.07601200
H	3.03734400	-1.46367800	-1.26161200
H	2.95445500	-1.34191800	1.52195300
N	-1.93614400	-0.51580900	0.04470100
O	-2.50716800	0.09987900	0.94690100
O	-2.48136700	-1.22610700	-0.79741700
S	1.69720800	1.19434200	-0.06214900
H	-0.24525100	-2.45455400	0.07378600
C	-0.85716000	2.11382300	-0.21657600
H	-1.61722000	1.90318600	-0.97156400
H	-1.38442500	2.27072500	0.72534900
H	-0.30636400	3.00995000	-0.48517400
Al	2.27594500	-1.17436000	0.09901800

Al(Tr-9)

C	0.01095900	1.07926600	0.06418000
C	-0.50395200	-0.16917400	-0.03100800
C	0.31110500	-1.35273800	-0.09780400
H	2.66649800	1.35779400	1.50758300
H	2.68657800	1.59402100	-1.27340300
C	-0.82374600	2.31235800	0.15529600
H	-1.02413000	2.66534000	-0.86118600
H	-1.79406900	2.15144200	0.62425900
H	-0.29005300	3.10623700	0.67504100
H	-0.20317800	-2.30810800	-0.14490300
N	-1.95211100	-0.45424300	-0.01764700
O	-2.31784700	-1.45747700	0.59802700
O	-2.69138800	0.33112600	-0.60855600
S	1.95190000	-1.34812400	-0.11776000
Al	2.03849400	1.07503900	0.07850300

Al(Tr-10)

C	0.29933200	-1.51408000	0.05405400
C	-0.46302600	-0.40860300	0.00519400
C	0.06800000	0.95051200	-0.07582600
H	3.03741300	-1.46295100	-1.26208000
H	2.95542700	-1.34121300	1.52133700
H	-0.24441600	-2.45491400	0.07510700
C	-0.85842100	2.11290900	-0.21565100
H	-1.61840500	1.90188200	-0.97062900
H	-1.38579100	2.26872000	0.72641100
H	-0.30861600	3.00972600	-0.48383900
N	-1.93582300	-0.51604000	0.04451800
O	-2.50652100	0.09636500	0.94916300
O	-2.48128200	-1.22284300	-0.80039400
S	1.69682600	1.19489600	-0.06235600
Al	2.27638800	-1.17383900	0.09869100

Al(Tr-11)

C	1.60812400	0.80547800	-0.07127200
C	0.27421200	1.08809700	-0.07906800
C	-0.66479800	0.01320300	-0.00424400
H	2.53388800	-1.63188600	1.51286000
H	2.53525700	-1.84025200	-1.26808900
H	-0.13453000	2.09201600	-0.14177300
C	2.58434900	1.93021500	-0.17045700
H	3.22993500	1.78535400	-1.04033800
H	2.10909000	2.90959700	-0.24278300
H	3.24858800	1.92299300	0.69735400

S	-0.37447000	-1.59933500	0.09683100
N	-2.10559300	0.42951800	-0.01137300
O	-2.35827200	1.48218700	0.57302400
O	-2.90709600	-0.30255900	-0.58173400
Al	2.04000500	-1.16262100	0.07946200

Al(Tr-12)

C	0.45821500	-0.23877800	0.01684400
C	0.06898400	1.06640700	-0.05656700
C	-1.35401300	1.30069900	-0.05707600
H	-1.12703900	-2.38059200	1.47374000
H	-1.17212100	-2.42380500	-1.32691400
N	1.89056900	-0.45728400	0.02338200
O	2.39001200	-0.88315300	-1.01862100
O	2.49540800	-0.21863600	1.06903300
S	-2.53419900	0.15546500	0.02103200
H	-1.68481400	2.33641600	-0.11006100
C	0.98157300	2.25762100	-0.12120300
H	1.03594400	2.74445200	0.85330100
H	1.99059300	1.97191900	-0.40989600
H	0.60893400	2.98359500	-0.84308400
Al	-0.95001600	-1.69383200	0.05903400

Al(Tr-13)

C	0.76858000	-0.07598100	-0.00139800
C	-0.15381300	-1.06365900	0.00199000
C	-1.55944800	-0.69842900	0.00136100
H	0.29996000	2.58423800	-1.40200000
H	0.28982600	2.57827900	1.40388100
C	-2.55050700	-1.81520400	0.00641100
H	-2.38098300	-2.44882300	-0.86708900
H	-2.38230200	-2.43914600	0.88719300
H	-3.57373200	-1.45248600	0.00386200
H	0.11700500	-2.11483500	0.00503400
N	2.17167500	-0.47433300	-0.00041200
O	2.97540600	0.47056700	0.01375000
O	2.48981500	-1.66539000	-0.01335600
S	-2.06352600	0.87426700	-0.00431900
Al	0.20725200	1.85408100	-0.00094100

Ga(Tr-0)

C	-0.13814000	1.52137700	-0.37185600
C	1.27128500	1.42120500	0.19975100
H	-0.62041400	2.42046400	0.01241900

H	-0.07571300	1.62991800	-1.45598200
C	1.87094300	0.06036500	0.08345800
H	1.98015200	2.13708100	-0.22833000
H	1.26323000	1.63388600	1.27929300
H	2.95225100	-0.02817400	0.16913200
H	-2.06605600	-0.77111800	-1.02661600
H	-1.44917900	-0.38344100	1.58401000
Ga	-1.17065600	-0.11935700	0.06724300
S	1.01759600	-1.30976500	-0.11791000

Ga(Tr-1)

C	-0.07404000	1.58643400	-0.00080700
C	1.27601300	1.44834600	0.00005000
H	-0.45489600	2.60373900	-0.00120600
C	1.85692600	0.12863500	0.00067000
H	1.96689300	2.28499600	0.00027100
H	2.94005000	0.03909900	0.00207700
H	-1.77998600	-0.48085900	-1.35476000
H	-1.77632400	-0.48163200	1.35683100
S	0.98716100	-1.26594600	-0.00058200
Ga	-1.13044200	-0.08679700	0.00021400

Ga(Tr-2)

C	0.95688000	1.57292600	-0.20793100
C	-0.39276200	1.43447900	-0.18887600
C	-0.93333100	0.11248200	-0.02619200
H	2.64842200	-0.30515000	1.42008600
H	2.64551100	-0.66513100	-1.27780700
H	1.33056500	2.58286800	-0.34910600
S	-0.10136400	-1.28422000	0.15253800
H	-1.10357500	2.24508600	-0.29109700
N	-2.42653900	0.02459800	-0.00881500
O	-3.00633200	0.97432400	0.51672200
O	-2.94687200	-0.97071100	-0.50101200
Ga	2.02992200	-0.07195400	0.01714000

Ga(Tr-3)

C	0.69162200	0.36828700	-0.00045500
C	0.21958300	1.63739100	0.00474800
C	-1.20906900	1.81185000	0.00528700
H	0.87013400	2.50396600	0.00858500
H	-1.60437900	2.82332500	0.01085100
H	-0.76521100	-1.84851500	1.37536700

H	-0.76017500	-1.85535000	-1.37530300
S	-2.29273600	0.57457500	-0.00179600
N	2.13584000	0.18531000	-0.00022100
O	2.51227300	-0.99557100	0.01160300
O	2.88733200	1.16333200	-0.01171600
Ga	-0.56184300	-1.17293700	-0.00147700

Ga(Tr-4)

C	0.15319500	-1.10598400	-0.00034500
C	0.98460600	-0.05169100	-0.00068900
C	0.51052200	1.31448900	-0.00095200
H	1.24405100	2.11231200	0.00055800
H	-2.48921400	-0.81878300	1.36832100
H	-2.49641700	-0.82854100	-1.35997900
H	0.62779900	-2.08185900	0.00004500
N	2.46290800	-0.21899800	0.00008400
O	3.14272300	0.80775000	0.00755900
O	2.90396500	-1.36149200	-0.00640600
S	-1.08142600	1.68588400	-0.00335000
Ga	-1.77700600	-0.65597500	0.00150800

Ga(Tr-5)

C	0.41539300	1.58158900	-0.00125700
C	-0.92926200	1.42357600	-0.00065400
C	-1.51917000	0.09824600	-0.00017900
H	2.16018300	-0.44998100	1.35723400
H	2.16856900	-0.45102300	-1.35131000
H	0.77906100	2.60540400	-0.00173300
H	-1.62850300	2.25597600	-0.00055600
C	-3.01117400	0.00472900	0.00131700
H	-3.40300300	0.52154400	0.88006200
H	-3.40476100	0.52389000	-0.87528300
H	-3.35530100	-1.02495500	0.00026700
S	-0.59718300	-1.27059900	-0.00126100
Ga	1.50012800	-0.07419700	0.00052100

Ga(Tr-6)

C	1.17543100	0.51989800	-0.00030000
C	0.47655400	1.68746900	0.00026700
C	-0.95527900	1.67553500	0.00063700
H	-0.01305200	-1.87341700	1.35882500
H	-0.01131000	-1.87802300	-1.35573100
H	-1.47725100	2.62913700	0.00200400
H	0.96368600	2.66007600	0.00072400

C	2.66637500	0.54203300	-0.00052300
H	3.04832300	0.00701700	-0.87307600
H	3.07973500	1.55212900	0.00072100
H	3.04886000	0.00458500	0.87028500
S	-1.88817700	0.31579800	-0.00077700
Ga	0.04494700	-1.11948000	0.00026400

Ga(Tr-7)

C	0.53735100	-1.21918500	-0.00084700
C	1.54391800	-0.30364700	-0.00014200
C	1.18021400	1.09726000	0.00048800
H	-2.07436900	-0.61983400	1.35664200
H	-2.08076900	-0.62408900	-1.35161100
H	0.84403800	-2.26297900	-0.00117000
S	-0.35536800	1.68092800	-0.00058500
H	1.98513600	1.83066100	0.00228200
C	3.01609900	-0.61943400	0.00007700
H	3.17558600	-1.69500300	-0.00156400
H	3.50479600	-0.19708500	-0.87906800
H	3.50399300	-0.19988100	0.88102100
Ga	-1.31735500	-0.54376200	0.00017300

Ga(Tr-8)

C	0.14719200	-1.28523100	0.03202500
C	-0.81713800	-0.35179700	-0.00421600
C	-0.55275200	1.08105000	-0.07758800
H	2.76617700	-0.71961200	-1.28725400
H	2.70495000	-0.62114200	1.43659700
N	-2.23733800	-0.74784200	0.04240400
O	-2.91781500	-0.24989200	0.94127500
O	-2.63287200	-1.55893500	-0.79242900
S	1.00411400	1.61389000	-0.08096100
H	-0.18973800	-2.31723900	0.05114000
C	-1.67870000	2.05494200	-0.19515500
H	-2.39438300	1.71674500	-0.94706900
H	-2.21624800	2.10330000	0.75247600
H	-1.30414500	3.03946700	-0.45787700
Ga	2.00138100	-0.59071100	0.05578600

Ga(Tr-9)

C	-0.17534500	0.92203400	0.04649200
C	-0.91864800	-0.20480100	-0.03518900
C	-0.33684000	-1.51784400	-0.09952900
H	2.46010700	0.71513000	1.43493800

H	2.49355400	0.92639400	-1.28472500
C	-0.74698900	2.29454300	0.13211800
H	-0.92471400	2.65902200	-0.88408900
H	-1.70808900	2.33126600	0.64432800
H	-0.04824500	2.97956000	0.60823700
H	-1.01430100	-2.36512400	-0.13820800
N	-2.39226400	-0.20602400	-0.01193400
O	-2.94113300	-1.13192200	0.58860900
O	-2.97068400	0.71851600	-0.58085700
S	1.27768700	-1.79670700	-0.12865800
Ga	1.78729100	0.55764200	0.04633000

Ga(Tr-10)

C	0.14701200	-1.28517400	0.03120800
C	-0.81724500	-0.35165800	-0.00473200
C	-0.55281800	1.08115700	-0.07796600
H	2.76700100	-0.71837900	-1.28645600
H	2.70401300	-0.62308600	1.43710000
H	-0.19010900	-2.31708700	0.05112500
C	-1.67821300	2.05548100	-0.19647100
H	-2.39419600	1.71712800	-0.94793300
H	-2.21566200	2.10507900	0.75116400
H	-1.30298600	3.03957900	-0.45983600
N	-2.23728200	-0.74791200	0.04265800
O	-2.91824500	-0.24783900	0.94005100
O	-2.63240300	-1.56140400	-0.79009000
S	1.00423600	1.61387600	-0.08011700
Ga	2.00122300	-0.59079900	0.05568300

Ga(Tr-11)

C	1.05975400	1.18700400	-0.07502700
C	-0.29951100	1.26284100	-0.07417200
C	-1.05625900	0.05358700	-0.00888200
H	2.35256400	-1.06501200	1.43234200
H	2.35724600	-1.22968100	-1.28723500
H	-0.85486900	2.19356100	-0.12322900
C	1.86955700	2.43455300	-0.16255500
H	2.51989700	2.39468000	-1.03968800
H	1.26155100	3.33836600	-0.21469500
H	2.53643500	2.50633600	0.69995600
S	-0.49545100	-1.48516700	0.07205000
N	-2.54686600	0.22678500	-0.00684300
O	-2.96574700	1.26716400	0.49973800
O	-3.22529200	-0.67131400	-0.49401600

Ga	1.79579100	-0.65670300	0.04211900

Ga(Tr-12)

C	0.61738500	-0.05876300	0.00412000
C	0.50676600	1.29805700	-0.04845500
C	-0.83679800	1.81438600	-0.05124700
H	-1.34189200	-1.80612800	1.41780900
H	-1.36655100	-1.84119900	-1.32711800
N	1.96757800	-0.57735700	0.01065900
O	2.38377800	-1.05599800	-1.04465300
O	2.59122800	-0.51278800	1.07055100
S	-2.21366800	0.91459300	0.00218900
H	-0.95820000	2.89484400	-0.08841200
C	1.65298400	2.26704600	-0.08688300
H	1.84677600	2.66321900	0.91047100
H	2.56426300	1.78916200	-0.44052100
H	1.42550700	3.10270500	-0.74722600
Ga	-1.03117200	-1.18608600	0.03396700

Ga(Tr-13)

C	0.70811400	0.44018300	-0.00063600
C	-0.26322500	1.37896900	0.00124600
C	-1.64524100	0.94347300	0.00108000
H	0.36718700	-2.19222800	1.37372600
H	0.37144800	-2.19456600	-1.37379800
C	-2.69728800	2.00328000	0.00383500
H	-2.56539100	2.63836000	0.88260300
H	-2.56641000	2.64193900	-0.87242500
H	-3.69773500	1.58172200	0.00360300
H	-0.04252100	2.44141600	0.00284200
N	2.08995000	0.90255200	0.00003800
O	2.94185300	0.00260100	0.01016100
O	2.34413000	2.10960500	-0.00939300
S	-2.05776700	-0.65496500	-0.00195700
Ga	0.24277500	-1.49187500	-0.00080000

In(Tr-0)

C	0.28729100	1.61669100	-0.39339300
C	1.66269500	1.38906200	0.21687200
H	-0.12325500	2.55443500	-0.01928000
H	0.37954800	1.71225900	-1.47628800
C	2.20202200	0.00052800	0.11063000
H	2.43270800	2.05973700	-0.18055800
H	1.64102500	1.59429500	1.29791800

H	3.27805000	-0.11166900	0.23598800
H	-2.00071000	-0.73152800	-1.20873300
H	-1.37452300	-0.37533100	1.70584000
S	1.34437800	-1.36140900	-0.12838700
In	-1.03377400	-0.06035400	0.04274800

In(Tr-1)

C	-0.33140800	1.67426200	-0.00010000
C	-1.66477400	1.42907100	-0.00064100
H	-0.04656500	2.72318500	0.00101200
C	-2.19480000	0.08475300	0.00038900
H	-2.40633300	2.22253500	-0.00105400
H	-3.27746800	-0.01911300	0.00238700
H	1.68846100	-0.47700300	1.50607800
H	1.69189900	-0.47839600	-1.50457700
In	0.99499900	-0.04343500	0.00003700
S	-1.32869200	-1.31071300	-0.00022100

In(Tr-2)

C	0.49377100	1.65537200	-0.25357200
C	-0.84211200	1.43247800	-0.21428200
C	-1.35139200	0.09740300	-0.02822900
H	2.46606400	-0.27081000	1.57828700
H	2.47598000	-0.73407400	-1.40715000
H	0.78615100	2.68949000	-0.41612700
S	-0.54628900	-1.30875400	0.17286000
H	-1.59009400	2.21028300	-0.31981800
N	-2.84614700	0.01810100	-0.00614900
O	-3.40597400	0.88047800	0.66894000
O	-3.38190000	-0.88250600	-0.64201500
In	1.81687600	-0.04442500	0.01231000

In(Tr-3)

C	-0.89310900	0.52159400	-0.00022800
C	-0.58626600	1.83829300	0.00018700
C	0.80097800	2.23594900	0.00026700
H	-1.35155200	2.60682700	0.00046800
H	1.00826600	3.30280400	0.00034800
H	0.98337400	-1.69970300	-1.52900400
H	0.98295900	-1.69866600	1.52962000
S	2.10120800	1.23114900	-0.00017500
N	-2.30604500	0.16365100	-0.00010200
O	-2.53240400	-1.05648600	0.00016600
O	-3.17728500	1.03653500	-0.00021200

In	0.62546600	-1.03613500	0.00002200

In(Tr-4)

C	-0.44132800	-1.05208400	0.00088100
C	-1.34927800	-0.06535100	-0.00007400
C	-1.03274400	1.34903500	-0.00100600
H	-1.86932000	2.03872900	-0.00108300
H	2.42928500	-0.49551200	-1.51681600
H	2.42830100	-0.49027900	1.51878200
H	-0.85542500	-2.05588500	0.00169600
N	-2.81350100	-0.37249800	0.00007400
O	-3.59001700	0.58293700	0.00640800
O	-3.14484700	-1.55125600	-0.00574300
In	1.64636000	-0.43694600	0.00063300
S	0.48181500	1.96110800	-0.00239100

In(Tr-5)

C	0.00989400	1.66981100	-0.00025600
C	1.33993900	1.42334800	-0.00044100
C	1.89810700	0.08054500	-0.00013100
H	-2.03360500	-0.46850600	-1.50161600
H	-2.03016000	-0.46842600	1.50420900
H	-0.27166300	2.71981000	-0.00047100
H	2.07814200	2.22282500	-0.00087500
C	3.39194400	-0.01583000	0.00064000
H	3.78617100	0.50239500	-0.87637100
H	3.78506500	0.50181700	0.87854300
H	3.73351400	-1.04625900	0.00067300
In	-1.32211300	-0.04359000	0.00011500
S	0.99354900	-1.29843600	-0.00053600

In(Tr-6)

C	1.13866900	0.92603100	-0.00021000
C	0.31145300	2.00457000	0.00005500
C	-1.11896300	1.89162100	0.00022400
H	0.07470500	-1.82903300	1.50663500
H	0.07523400	-1.83088900	-1.50526000
H	-1.68275200	2.82194900	0.00074200
H	0.70578000	3.01976100	0.00026100
C	2.61601700	1.13682900	-0.00014300
H	3.06446700	0.65433100	-0.87188700
H	2.89815800	2.19222700	-0.00003300
H	3.06430900	0.65425700	0.87167100
In	0.12867600	-1.01113600	0.00004200

S	-2.01175400	0.50679900	-0.00023200

In(Tr-7)

C	0.73092900	-1.24661800	-0.00022200
C	1.83267400	-0.45065600	-0.00005500
C	1.68165200	0.99236700	0.00016200
H	-2.04720300	-0.23232800	1.50202100
H	-2.04846000	-0.23299100	-1.50114700
H	0.93234000	-2.31625400	-0.00030600
S	0.28681900	1.85798400	-0.00014800
H	2.60283900	1.57453200	0.00059800
C	3.25525600	-0.95132600	0.00002900
H	3.27816800	-2.03844000	-0.00022200
H	3.79310100	-0.59487200	-0.87983100
H	3.79280900	-0.59529200	0.88023900
In	-1.22236300	-0.31336100	0.00003100

In(Tr-8)

C	-0.13078700	-1.23083400	0.00700000
C	-1.15365900	-0.36393100	-0.00934200
C	-1.04180700	1.09179600	-0.06984300
H	2.65670000	-0.35586400	-1.46807700
H	2.60479300	-0.30800800	1.55640900
N	-2.53996400	-0.87279500	0.04453800
O	-3.20446200	-0.55010100	1.03093700
O	-2.92326200	-1.59263100	-0.87619000
S	0.42519700	1.83398500	-0.07516400
H	-0.41625100	-2.27888000	0.01575600
C	-2.28562500	1.91519900	-0.16938600
H	-2.94961900	1.50608600	-0.93398600
H	-2.82616800	1.87079100	0.77715000
H	-2.04132400	2.94579900	-0.40609800
In	1.84982700	-0.36623800	0.03186000

In(Tr-9)

C	0.45626400	-0.89207300	0.04700200
C	1.27617800	0.17742500	-0.03400100
C	0.84681800	1.55154200	-0.09596400
H	-2.43631600	-0.39634800	1.56319900
H	-2.45889200	-0.63482600	-1.46180300
C	0.94250800	-2.29884900	0.13045200
H	0.95724100	-2.71564300	-0.88165700
H	1.95335400	-2.39725800	0.52525900

H	0.25873300	-2.91079200	0.71677700
H	1.63576000	2.29819500	-0.11859600
N	2.74831000	0.04503000	-0.00844000
O	3.36730500	0.84266000	0.69879300
O	3.25112100	-0.85499500	-0.67959800
In	-1.67302300	-0.36576600	0.03307900
S	-0.70299600	2.07715100	-0.14646700

In(Tr-10)

C	-0.13300300	-1.22935400	0.00398300
C	-1.15817000	-0.36441800	-0.01062400
C	-1.05349100	1.09269200	-0.07128800
H	2.67726800	-0.34549500	-1.47063100
H	2.62082800	-0.30729600	1.56177000
H	-0.41122300	-2.27968600	0.01285700
C	-2.30299300	1.90810600	-0.17492400
H	-2.96583900	1.48954300	-0.93528000
H	-2.84162600	1.86741000	0.77282000
H	-2.06557800	2.93855000	-0.41948600
N	-2.54248500	-0.88056400	0.04578100
O	-3.21136900	-0.55010200	1.02666600
O	-2.91907000	-1.61486100	-0.86622100
In	1.86090800	-0.36429100	0.03188000
S	0.40803200	1.84554400	-0.07319100

In(Tr-11)

C	0.56002600	1.43347400	-0.09722400
C	-0.79205300	1.29523200	-0.08191700
C	-1.40757200	0.00526800	-0.00949500
H	2.32794900	-0.81791400	1.57446300
H	2.33406800	-1.01930100	-1.44217700
H	-1.46926900	2.14366900	-0.12564400
C	1.14668700	2.80090900	-0.19765600
H	1.78739700	2.86793000	-1.08041300
H	0.39334900	3.58920500	-0.24873200
H	1.79798700	2.99113600	0.65896100
S	-0.73821600	-1.48641200	0.07355700
N	-2.90837500	0.05236500	0.00003300
O	-3.40735400	0.94466900	0.68417200
O	-3.50979300	-0.79095200	-0.65584800
In	1.69986200	-0.42403500	0.03219500

In(Tr-12)

C	0.85247800	-0.05129800	0.01015400
C	1.08885500	1.28762100	-0.04994400
C	-0.05554400	2.16684300	-0.04922000
H	-1.73439900	-1.36355300	1.55214100
H	-1.74801500	-1.34638700	-1.50842000
N	2.02851800	-0.89199400	0.01456000
O	2.28525100	-1.49235600	-1.03042800
O	2.67124000	-0.96536800	1.06306900
S	-1.64773400	1.76065500	0.00447800
H	0.16222200	3.23312100	-0.08556500
C	2.44959100	1.92576200	-0.10069500
H	2.72763300	2.30190800	0.88456200
H	3.21239100	1.21739100	-0.41617800
H	2.45034500	2.76355700	-0.79704000
In	-1.19531200	-0.83764000	0.02191900

In(Tr-13)

C	0.48442700	0.86782600	-0.00017900
C	-0.67413400	1.55895500	0.00000400
C	-1.94607900	0.85642900	-0.00001400
H	0.79595700	-2.02542500	1.52749000
H	0.79556400	-2.02557100	-1.52768800
C	-3.17058500	1.71486000	0.00019900
H	-3.15355300	2.36478800	0.87802700
H	-3.15320800	2.36586000	-0.87684400
H	-4.08032300	1.12258500	-0.00029700
H	-0.68761700	2.64495400	0.00013200
N	1.72156600	1.64114000	-0.00001200
O	2.75921700	0.96101700	0.00079600
O	1.69566500	2.87439200	-0.00057500
In	0.55144900	-1.30652600	-0.00006500
S	-2.08685200	-0.78669400	0.00003700