

Differences in Acetone

optS0

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	5.32e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	5.32e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.04e-01	2.73e-01	2.74e-01	2.74e-01
BDP-Ph	1.04e-01	0.00e+00	2.61e-01	2.61e-01	2.60e-01
BDP-PPPh	2.73e-01	2.61e-01	0.00e+00	2.74e-02	2.84e-02
OMe-out	2.74e-01	2.61e-01	2.74e-02	0.00e+00	3.09e-03
OMe-in	2.74e-01	2.60e-01	2.84e-02	3.09e-03	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.62e-01	2.90e-01	2.89e-01
BDP-Ph	1.05e-01	0.00e+00	2.42e-01	2.77e-01	2.76e-01
BDP-PPPh	2.62e-01	2.42e-01	0.00e+00	5.43e-02	5.12e-02
OMe-out	2.90e-01	2.77e-01	5.43e-02	0.00e+00	8.61e-03
OMe-in	2.89e-01	2.76e-01	5.12e-02	8.61e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	2.69e+01	3.58e+01	2.87e+01	2.60e+01
BDP-Ph	2.69e+01	0.00e+00	4.12e+01	3.78e+01	3.18e+01
BDP-PPPh	3.58e+01	4.12e+01	0.00e+00	3.84e+01	3.21e+01
OMe-out	2.87e+01	3.78e+01	3.84e+01	0.00e+00	2.22e+01
OMe-in	2.60e+01	3.18e+01	3.21e+01	2.22e+01	0.00e+00

optS1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	4.94e-07
OMe-in	3.03e+01	4.31e+01	1.43e+01	4.94e-07	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.26e-01	7.85e-01	8.68e-01	8.78e-01
BDP-Ph	1.26e-01	0.00e+00	7.61e-01	8.34e-01	8.45e-01
BDP-PPPh	7.85e-01	7.61e-01	0.00e+00	1.72e-01	1.79e-01
OMe-out	8.68e-01	8.34e-01	1.72e-01	0.00e+00	1.19e-02
OMe-in	8.78e-01	8.45e-01	1.79e-01	1.19e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.07e-01	3.58e-01	3.90e-01	3.90e-01
BDP-Ph	1.07e-01	0.00e+00	3.82e-01	4.10e-01	4.10e-01
BDP-PPPh	3.58e-01	3.82e-01	0.00e+00	1.10e-01	1.10e-01
OMe-out	3.90e-01	4.10e-01	1.10e-01	0.00e+00	7.57e-03
OMe-in	3.90e-01	4.10e-01	1.10e-01	7.57e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.55e+01	3.83e+01	3.62e+01	3.57e+01
BDP-Ph	1.55e+01	0.00e+00	3.81e+01	3.68e+01	3.55e+01
BDP-PPPh	3.83e+01	3.81e+01	0.00e+00	8.52e+00	8.73e+00
OMe-out	3.62e+01	3.68e+01	8.52e+00	0.00e+00	2.76e+00
OMe-in	3.57e+01	3.55e+01	8.73e+00	2.76e+00	0.00e+00

optR1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	3.69e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	3.69e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.20e-01	7.62e-01	8.65e-01	8.76e-01
BDP-Ph	1.20e-01	0.00e+00	7.25e-01	8.13e-01	8.23e-01
BDP-PPPh	7.62e-01	7.25e-01	0.00e+00	1.72e-01	1.81e-01
OMe-out	8.65e-01	8.13e-01	1.72e-01	0.00e+00	1.52e-02
OMe-in	8.76e-01	8.23e-01	1.81e-01	1.52e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.01e-01	4.61e-01	5.96e-01	5.90e-01
BDP-Ph	1.01e-01	0.00e+00	4.93e-01	6.25e-01	6.20e-01
BDP-PPPh	4.61e-01	4.93e-01	0.00e+00	1.70e-01	1.64e-01
OMe-out	5.96e-01	6.25e-01	1.70e-01	0.00e+00	1.93e-02
OMe-in	5.90e-01	6.20e-01	1.64e-01	1.93e-02	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.28e+01	1.28e+02	1.22e+02	1.23e+02
BDP-Ph	1.28e+01	0.00e+00	1.26e+02	1.21e+02	1.22e+02
BDP-PPPh	1.28e+02	1.26e+02	0.00e+00	3.32e+01	3.07e+01
OMe-out	1.22e+02	1.21e+02	3.32e+01	0.00e+00	1.05e+01
OMe-in	1.23e+02	1.22e+02	3.07e+01	1.05e+01	0.00e+00

Differences in DiMethylFormamide

optS0

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	4.50e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	4.50e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.74e-01	2.75e-01	2.75e-01
BDP-Ph	1.05e-01	0.00e+00	2.62e-01	2.62e-01	2.61e-01
BDP-PPPh	2.74e-01	2.62e-01	0.00e+00	2.74e-02	2.85e-02
OMe-out	2.75e-01	2.62e-01	2.74e-02	0.00e+00	3.59e-03
OMe-in	2.75e-01	2.61e-01	2.85e-02	3.59e-03	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.62e-01	2.91e-01	2.89e-01
BDP-Ph	1.05e-01	0.00e+00	2.42e-01	2.77e-01	2.75e-01
BDP-PPPh	2.62e-01	2.42e-01	0.00e+00	5.39e-02	5.05e-02
OMe-out	2.91e-01	2.77e-01	5.39e-02	0.00e+00	9.37e-03
OMe-in	2.89e-01	2.75e-01	5.05e-02	9.37e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	2.57e+01	3.63e+01	2.88e+01	2.64e+01
BDP-Ph	2.57e+01	0.00e+00	4.03e+01	3.80e+01	3.24e+01
BDP-PPPh	3.63e+01	4.03e+01	0.00e+00	3.76e+01	3.15e+01
OMe-out	2.88e+01	3.80e+01	3.76e+01	0.00e+00	2.26e+01
OMe-in	2.64e+01	3.24e+01	3.15e+01	2.26e+01	0.00e+00

optS1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	8.35e-07
OMe-in	3.03e+01	4.31e+01	1.43e+01	8.35e-07	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.25e-01	7.86e-01	8.69e-01	8.80e-01
BDP-Ph	1.25e-01	0.00e+00	7.63e-01	8.36e-01	8.47e-01
BDP-PPPh	7.86e-01	7.63e-01	0.00e+00	1.73e-01	1.80e-01
OMe-out	8.69e-01	8.36e-01	1.73e-01	0.00e+00	1.18e-02
OMe-in	8.80e-01	8.47e-01	1.80e-01	1.18e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.07e-01	3.59e-01	3.90e-01	3.90e-01
BDP-Ph	1.07e-01	0.00e+00	3.83e-01	4.11e-01	4.11e-01
BDP-PPPh	3.59e-01	3.83e-01	0.00e+00	1.08e-01	1.09e-01
OMe-out	3.90e-01	4.11e-01	1.08e-01	0.00e+00	7.76e-03
OMe-in	3.90e-01	4.11e-01	1.09e-01	7.76e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.56e+01	3.85e+01	3.65e+01	3.59e+01
BDP-Ph	1.56e+01	0.00e+00	3.81e+01	3.73e+01	3.59e+01
BDP-PPPh	3.85e+01	3.81e+01	0.00e+00	8.36e+00	8.56e+00
OMe-out	3.65e+01	3.73e+01	8.36e+00	0.00e+00	2.84e+00
OMe-in	3.59e+01	3.59e+01	8.56e+00	2.84e+00	0.00e+00

optR1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	3.51e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	3.51e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.20e-01	7.63e-01	8.67e-01	8.77e-01
BDP-Ph	1.20e-01	0.00e+00	7.28e-01	8.15e-01	8.26e-01
BDP-PPPh	7.63e-01	7.28e-01	0.00e+00	1.73e-01	1.82e-01
OMe-out	8.67e-01	8.15e-01	1.73e-01	0.00e+00	1.54e-02
OMe-in	8.77e-01	8.26e-01	1.82e-01	1.54e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.00e-01	4.58e-01	5.92e-01	5.86e-01
BDP-Ph	1.00e-01	0.00e+00	4.89e-01	6.21e-01	6.15e-01
BDP-PPPh	4.58e-01	4.89e-01	0.00e+00	1.70e-01	1.64e-01
OMe-out	5.92e-01	6.21e-01	1.70e-01	0.00e+00	2.00e-02
OMe-in	5.86e-01	6.15e-01	1.64e-01	2.00e-02	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.26e+01	1.28e+02	1.22e+02	1.23e+02
BDP-Ph	1.26e+01	0.00e+00	1.26e+02	1.21e+02	1.22e+02
BDP-PPPh	1.28e+02	1.26e+02	0.00e+00	2.93e+01	2.84e+01
OMe-out	1.22e+02	1.21e+02	2.93e+01	0.00e+00	9.94e+00
OMe-in	1.23e+02	1.22e+02	2.84e+01	9.94e+00	0.00e+00

Differences in DiMethylSulfoxide

optS0

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	4.29e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	4.29e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.74e-01	2.75e-01	2.75e-01
BDP-Ph	1.05e-01	0.00e+00	2.62e-01	2.62e-01	2.61e-01
BDP-PPPh	2.74e-01	2.62e-01	0.00e+00	2.73e-02	2.85e-02
OMe-out	2.75e-01	2.62e-01	2.73e-02	0.00e+00	3.65e-03
OMe-in	2.75e-01	2.61e-01	2.85e-02	3.65e-03	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.63e-01	2.91e-01	2.89e-01
BDP-Ph	1.05e-01	0.00e+00	2.42e-01	2.77e-01	2.75e-01
BDP-PPPh	2.63e-01	2.42e-01	0.00e+00	5.39e-02	5.04e-02
OMe-out	2.91e-01	2.77e-01	5.39e-02	0.00e+00	9.55e-03
OMe-in	2.89e-01	2.75e-01	5.04e-02	9.55e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	2.55e+01	3.65e+01	2.89e+01	2.64e+01
BDP-Ph	2.55e+01	0.00e+00	4.00e+01	3.80e+01	3.25e+01
BDP-PPPh	3.65e+01	4.00e+01	0.00e+00	3.74e+01	3.13e+01
OMe-out	2.89e+01	3.80e+01	3.74e+01	0.00e+00	2.26e+01
OMe-in	2.64e+01	3.25e+01	3.13e+01	2.26e+01	0.00e+00

optS1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	9.23e-07
OMe-in	3.03e+01	4.31e+01	1.43e+01	9.23e-07	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.24e-01	7.86e-01	8.69e-01	8.80e-01
BDP-Ph	1.24e-01	0.00e+00	7.63e-01	8.37e-01	8.48e-01
BDP-PPPh	7.86e-01	7.63e-01	0.00e+00	1.73e-01	1.80e-01
OMe-out	8.69e-01	8.37e-01	1.73e-01	0.00e+00	1.19e-02
OMe-in	8.80e-01	8.48e-01	1.80e-01	1.19e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.06e-01	3.59e-01	3.90e-01	3.90e-01
BDP-Ph	1.06e-01	0.00e+00	3.82e-01	4.12e-01	4.12e-01
BDP-PPPh	3.59e-01	3.82e-01	0.00e+00	1.08e-01	1.08e-01
OMe-out	3.90e-01	4.12e-01	1.08e-01	0.00e+00	7.88e-03
OMe-in	3.90e-01	4.12e-01	1.08e-01	7.88e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.56e+01	3.85e+01	3.66e+01	3.60e+01
BDP-Ph	1.56e+01	0.00e+00	3.81e+01	3.75e+01	3.60e+01
BDP-PPPh	3.85e+01	3.81e+01	0.00e+00	8.32e+00	8.51e+00
OMe-out	3.66e+01	3.75e+01	8.32e+00	0.00e+00	2.86e+00
OMe-in	3.60e+01	3.60e+01	8.51e+00	2.86e+00	0.00e+00

optR1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	3.46e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	3.46e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.20e-01	7.63e-01	8.67e-01	8.78e-01
BDP-Ph	1.20e-01	0.00e+00	7.28e-01	8.16e-01	8.27e-01
BDP-PPPh	7.63e-01	7.28e-01	0.00e+00	1.73e-01	1.82e-01
OMe-out	8.67e-01	8.16e-01	1.73e-01	0.00e+00	1.55e-02
OMe-in	8.78e-01	8.27e-01	1.82e-01	1.55e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	9.99e-02	4.57e-01	5.91e-01	5.85e-01
BDP-Ph	9.99e-02	0.00e+00	4.87e-01	6.19e-01	6.14e-01
BDP-PPPh	4.57e-01	4.87e-01	0.00e+00	1.70e-01	1.64e-01
OMe-out	5.91e-01	6.19e-01	1.70e-01	0.00e+00	2.02e-02
OMe-in	5.85e-01	6.14e-01	1.64e-01	2.02e-02	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.26e+01	1.28e+02	1.22e+02	1.23e+02
BDP-Ph	1.26e+01	0.00e+00	1.26e+02	1.21e+02	1.22e+02
BDP-PPPh	1.28e+02	1.26e+02	0.00e+00	2.86e+01	2.79e+01
OMe-out	1.22e+02	1.21e+02	2.86e+01	0.00e+00	9.85e+00
OMe-in	1.23e+02	1.22e+02	2.79e+01	9.85e+00	0.00e+00

Differences in Methanol

optS0

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	4.65e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	4.65e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.74e-01	2.75e-01	2.75e-01
BDP-Ph	1.05e-01	0.00e+00	2.62e-01	2.61e-01	2.60e-01
BDP-PPPh	2.74e-01	2.62e-01	0.00e+00	2.73e-02	2.85e-02
OMe-out	2.75e-01	2.61e-01	2.73e-02	0.00e+00	3.49e-03
OMe-in	2.75e-01	2.60e-01	2.85e-02	3.49e-03	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.62e-01	2.91e-01	2.89e-01
BDP-Ph	1.05e-01	0.00e+00	2.42e-01	2.77e-01	2.75e-01
BDP-PPPh	2.62e-01	2.42e-01	0.00e+00	5.40e-02	5.06e-02
OMe-out	2.91e-01	2.77e-01	5.40e-02	0.00e+00	9.26e-03
OMe-in	2.89e-01	2.75e-01	5.06e-02	9.26e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	2.59e+01	3.62e+01	2.87e+01	2.63e+01
BDP-Ph	2.59e+01	0.00e+00	4.04e+01	3.79e+01	3.22e+01
BDP-PPPh	3.62e+01	4.04e+01	0.00e+00	3.77e+01	3.16e+01
OMe-out	2.87e+01	3.79e+01	3.77e+01	0.00e+00	2.25e+01
OMe-in	2.63e+01	3.22e+01	3.16e+01	2.25e+01	0.00e+00

optS1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	7.79e-07
OMe-in	3.03e+01	4.31e+01	1.43e+01	7.79e-07	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.25e-01	7.86e-01	8.69e-01	8.79e-01
BDP-Ph	1.25e-01	0.00e+00	7.62e-01	8.36e-01	8.47e-01
BDP-PPPh	7.86e-01	7.62e-01	0.00e+00	1.73e-01	1.80e-01
OMe-out	8.69e-01	8.36e-01	1.73e-01	0.00e+00	1.18e-02
OMe-in	8.79e-01	8.47e-01	1.80e-01	1.18e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.07e-01	3.59e-01	3.90e-01	3.90e-01
BDP-Ph	1.07e-01	0.00e+00	3.82e-01	4.11e-01	4.11e-01
BDP-PPPh	3.59e-01	3.82e-01	0.00e+00	1.08e-01	1.09e-01
OMe-out	3.90e-01	4.11e-01	1.08e-01	0.00e+00	7.82e-03
OMe-in	3.90e-01	4.11e-01	1.09e-01	7.82e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.56e+01	3.84e+01	3.65e+01	3.59e+01
BDP-Ph	1.56e+01	0.00e+00	3.81e+01	3.73e+01	3.59e+01
BDP-PPPh	3.84e+01	3.81e+01	0.00e+00	8.37e+00	8.58e+00
OMe-out	3.65e+01	3.73e+01	8.37e+00	0.00e+00	2.82e+00
OMe-in	3.59e+01	3.59e+01	8.58e+00	2.82e+00	0.00e+00

optR1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	3.54e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	3.54e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.20e-01	7.63e-01	8.67e-01	8.77e-01
BDP-Ph	1.20e-01	0.00e+00	7.27e-01	8.15e-01	8.25e-01
BDP-PPPh	7.63e-01	7.27e-01	0.00e+00	1.73e-01	1.81e-01
OMe-out	8.67e-01	8.15e-01	1.73e-01	0.00e+00	1.54e-02
OMe-in	8.77e-01	8.25e-01	1.81e-01	1.54e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.00e-01	4.58e-01	5.93e-01	5.86e-01
BDP-Ph	1.00e-01	0.00e+00	4.89e-01	6.21e-01	6.16e-01
BDP-PPPh	4.58e-01	4.89e-01	0.00e+00	1.70e-01	1.64e-01
OMe-out	5.93e-01	6.21e-01	1.70e-01	0.00e+00	1.99e-02
OMe-in	5.86e-01	6.16e-01	1.64e-01	1.99e-02	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.26e+01	1.28e+02	1.22e+02	1.23e+02
BDP-Ph	1.26e+01	0.00e+00	1.26e+02	1.21e+02	1.22e+02
BDP-PPPh	1.28e+02	1.26e+02	0.00e+00	2.97e+01	2.87e+01
OMe-out	1.22e+02	1.21e+02	2.97e+01	0.00e+00	1.01e+01
OMe-in	1.23e+02	1.22e+02	2.87e+01	1.01e+01	0.00e+00

Differences in TetraHydroFuran

optS0

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	8.19e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	8.19e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.02e-01	2.70e-01	2.71e-01	2.71e-01
BDP-Ph	1.02e-01	0.00e+00	2.58e-01	2.58e-01	2.57e-01
BDP-PPPh	2.70e-01	2.58e-01	0.00e+00	2.75e-02	2.79e-02
OMe-out	2.71e-01	2.58e-01	2.75e-02	0.00e+00	2.26e-03
OMe-in	2.71e-01	2.57e-01	2.79e-02	2.26e-03	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.05e-01	2.61e-01	2.89e-01	2.88e-01
BDP-Ph	1.05e-01	0.00e+00	2.43e-01	2.78e-01	2.78e-01
BDP-PPPh	2.61e-01	2.43e-01	0.00e+00	5.60e-02	5.47e-02
OMe-out	2.89e-01	2.78e-01	5.60e-02	0.00e+00	7.26e-03
OMe-in	2.88e-01	2.78e-01	5.47e-02	7.26e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	3.11e+01	3.45e+01	2.84e+01	2.46e+01
BDP-Ph	3.11e+01	0.00e+00	4.23e+01	3.76e+01	3.02e+01
BDP-PPPh	3.45e+01	4.23e+01	0.00e+00	4.16e+01	3.54e+01
OMe-out	2.84e+01	3.76e+01	4.16e+01	0.00e+00	2.16e+01
OMe-in	2.46e+01	3.02e+01	3.54e+01	2.16e+01	0.00e+00

optS1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	7.06e-07
OMe-in	3.03e+01	4.31e+01	1.43e+01	7.06e-07	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.31e-01	7.83e-01	8.62e-01	8.73e-01
BDP-Ph	1.31e-01	0.00e+00	7.55e-01	8.25e-01	8.35e-01
BDP-PPPh	7.83e-01	7.55e-01	0.00e+00	1.70e-01	1.77e-01
OMe-out	8.62e-01	8.25e-01	1.70e-01	0.00e+00	1.21e-02
OMe-in	8.73e-01	8.35e-01	1.77e-01	1.21e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.11e-01	3.56e-01	3.90e-01	3.90e-01
BDP-Ph	1.11e-01	0.00e+00	3.80e-01	4.06e-01	4.07e-01
BDP-PPPh	3.56e-01	3.80e-01	0.00e+00	1.16e-01	1.14e-01
OMe-out	3.90e-01	4.06e-01	1.16e-01	0.00e+00	7.92e-03
OMe-in	3.90e-01	4.07e-01	1.14e-01	7.92e-03	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.54e+01	3.76e+01	3.52e+01	3.49e+01
BDP-Ph	1.54e+01	0.00e+00	3.80e+01	3.49e+01	3.40e+01
BDP-PPPh	3.76e+01	3.80e+01	0.00e+00	9.27e+00	9.48e+00
OMe-out	3.52e+01	3.49e+01	9.27e+00	0.00e+00	2.60e+00
OMe-in	3.49e+01	3.40e+01	9.48e+00	2.60e+00	0.00e+00

optR1

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.83e+01	1.87e+01	3.03e+01	3.03e+01
BDP-Ph	1.83e+01	0.00e+00	3.36e+01	4.31e+01	4.31e+01
BDP-PPPh	1.87e+01	3.36e+01	0.00e+00	1.43e+01	1.43e+01
OMe-out	3.03e+01	4.31e+01	1.43e+01	0.00e+00	4.35e-06
OMe-in	3.03e+01	4.31e+01	1.43e+01	4.35e-06	0.00e+00

RMS R

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.19e-01	7.58e-01	8.59e-01	8.70e-01
BDP-Ph	1.19e-01	0.00e+00	7.18e-01	8.03e-01	8.14e-01
BDP-PPPh	7.58e-01	7.18e-01	0.00e+00	1.70e-01	1.78e-01
OMe-out	8.59e-01	8.03e-01	1.70e-01	0.00e+00	1.44e-02
OMe-in	8.70e-01	8.14e-01	1.78e-01	1.44e-02	0.00e+00

RMS A

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.03e-01	4.75e-01	6.13e-01	6.08e-01
BDP-Ph	1.03e-01	0.00e+00	5.10e-01	6.45e-01	6.41e-01
BDP-PPPh	4.75e-01	5.10e-01	0.00e+00	1.71e-01	1.65e-01
OMe-out	6.13e-01	6.45e-01	1.71e-01	0.00e+00	1.70e-02
OMe-in	6.08e-01	6.41e-01	1.65e-01	1.70e-02	0.00e+00

RMS D

	BDP-NPh	BDP-Ph	BDP-PPPh	OMe-out	OMe-in
BDP-NPh	0.00e+00	1.35e+01	1.27e+02	1.22e+02	1.23e+02
BDP-Ph	1.35e+01	0.00e+00	1.25e+02	1.21e+02	1.22e+02
BDP-PPPh	1.27e+02	1.25e+02	0.00e+00	3.03e+01	3.55e+01
OMe-out	1.22e+02	1.21e+02	3.03e+01	0.00e+00	1.78e+01
OMe-in	1.23e+02	1.22e+02	3.55e+01	1.78e+01	0.00e+00